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PRELIMINARY SCORING OF SELECTED ORGANIC AIR POLLUTANTS APPENDIX II - CHEMISTRY, PRODUCTION, AND TOXICITY OF CHEMICALS D THROUGH E

U.S. ENVIRONMENTAL PROTECTION AGENCY
Office of Air and Waste Management
Office of Air Quality Planning and Standards
Research Triangle Park, North Carolina 27711

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by

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Office of Air and Waste Management
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PREFACE

A program is being developed by the Emission Standards and Engineering Division of the U.S. Environmental Protection Agency to determine the extent and environmental effects of atmospheric industrial emissions of synthetic organic chemicals. As part of the initial effort, EPA requested that the MITRE Corporation, METREK Division, devise a system for identifying those chemicals that may be released to the atmosphere from chemical manufacturing plants and whose health effects have been documented. To address this need, three general categories of information for each compound to be evaluated were deemed directly relevant:

(1) the quantity of the compound produced;

(2) the potential for atmospheric release from chemical manufacturing plants, and

(3) the toxicological effects of the compounds.

The results of this study are presented in the accompanying report "Preliminary Scoring of Organic Air Pollutants."

The following dossiers were prepared for each of the 637 compounds under consideration in an attempt to collate the pertinent data for subsequent evaluation.

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APPENDIX II

CHEMISTRY, PRODUCTION AND TOXICITY OF SELECTED SYNTHETIC ORGANIC CHEMICALS

Dacthal

CHEMICAL NAME

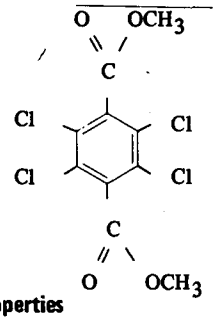
CAS Number: 1861-32-1

Chemical Name: 2,3,5,6-Tetrachloro-1,4-benzenedicarboxylic acid, dimethyl ester

Synonyms: Dimethyl-2,3,5,6-tetrachloroterephthalate
DCAP
Tetrachloroterephthalic acid, dimethyl ester

Molecular Formula: $C_{10}H_6Cl_4O_4$

Structure:



Chemical Properties

Molecular Weight: 332.0

Physical State: Solid

Vapor Pressure: <0.01 mm at 40°C

Vapor Density:

Boiling Point: (none) decomposes at 360 to 370°C

Melting Point: 156°C

Density: 1.70

Solubility: Very slightly soluble (H_2O) (0.5 ppm at 25°C)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Stable to ultraviolet irradiation

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 2.0×10^6 lbs.

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3000 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dalapon

CHEMICAL NAME

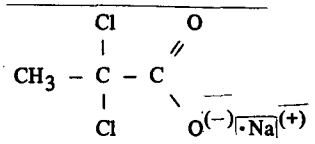
CAS Number: 127-20-8

Chemical Name: 2,2-Dichloropropionic acid, sodium salt

Synonyms: Dalapon

Molecular Formula: $C_3H_3Cl_2O_2 \cdot Na$

Structure:



Chemical Properties

Molecular Weight: 164.95

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 98°C at 20 mm

Melting Point: 174 to 176°C (decomposes)

Density:

Solubility: Soluble (H_2O) (45 gm/100 ml at 25°C) (hydrolyzes above 70°C)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 5×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 5.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	7500 to 9300 mg/kg	rat	oral
	3860 mg/kg	rat	oral

Low toxicity to man

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:
Irritant to eyes and skin

Dasanit

CHEMICAL NAME

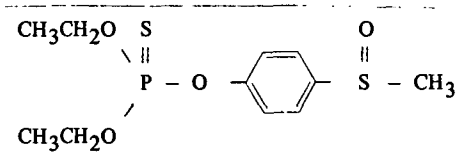
CAS Number: 115-90-2

Chemical Name: Phosophorothioic acid, O,O-diethyl-O-[p-(methylsulfinyl)phenyl] ester

Synonyms: Bayer S767
Dasanit

Molecular Formula: $C_{11}H_{17}O_4PS_2$

Structure:



Chemical Properties

Molecular Weight: 276.31

Physical State: Liquid

Vapor Pressure: <10 mm at 25°C

Vapor Density:

Boiling Point:

Melting Point:

Density:

Solubility:

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 4×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 4.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2 to 10 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

DBCP

CHEMICAL NAME

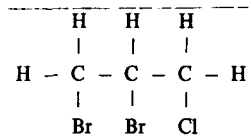
CAS Number: 96-12-8

Chemical Name: 1,2-Dibromo-3-chloropropane

Synonyms: Nemagon

Molecular Formula: $C_3H_5Br_2Cl$

Structure:



Chemical Properties

Molecular Weight: 236.35

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 195.5°C

Melting Point: 6.7°C

Density: 2.05 at 20°C

Solubility: Slightly (1000 ppm) (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 10×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 10.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	173 to 275 mg/kg	rat	oral

Non-lethal Acute Effects:

Irritant to skin and mucous membranes
Narcotic at high concentrations

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

DDT

CHEMICAL NAME

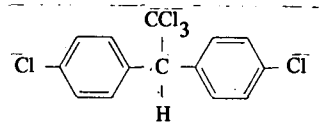
CAS Number: 50-29-3

Chemical Name: 1,1,1-Trichloro-2,2-bis(p-chlorophenyl)ethane

Synonyms: α-Bis (p-chlorophenyl) ββ-trichloroethane
Dichlorodiphenyltrichloroethane
Chlorophenothane
Dicophane

Molecular Formula: $C_{14}H_9Cl_5$

Structure:



Chemical Properties

Molecular Weight: 354.5

Physical State: Solid

Vapor Pressure: 1.9×10^{-7} Torrs at 20°C

Vapor Density:

Boiling Point: Decomposes

Melting Point: 108.5°C

Density:

Solubility: Practically insoluble (H_2O)

Octanol/Water Partition Coefficient: 4.96

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 45 x 10^6 lbs.

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 45

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	113 mg/kg	rat	oral
	2500 mg/kg	rat	skin
	1500 mg/kg	rat	subcutaneous
	135 mg/kg	mouse	oral
	280 mg/kg	mouse	intraperitoneal
	250 mg/kg	rabbit	oral
	300 mg/kg	rabbit	skin
	250 mg/kg	rabbit	subcutaneous
	1000 mg/kg	guinea pig	skin
	900 mg/kg	guinea pig	subcutaneous
	35 mg/kg	frog	subcutaneous
LD_{Lo}	31 mg/kg	infant	oral
	16 mg/kg	human	oral
	3 gm/kg	woman	oral
	113 mg/kg	rat	oral
	940 mg/kg	rat	intraperitoneal
	30 mg/kg	rat	intravenous
	73 mg/kg (26 wks)	mouse	oral
	75 mg/kg	dog	intravenous
	50 mg/kg	monkey	intravenous
	250 mg/kg	cat	oral
	40 mg/kg	cat	intravenous
	50 mg/kg	rabbit	intravenous
	224 mg/kg	guinea pig	oral

Chronic Toxicity

U.S. Occupational Standard: (air): TWA 1 mg/m^3 (skin)

Carcinogenicity: Causes tumors "indicative of cancer" in laboratory rats and mice

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Decahydronaphthalene

CHEMICAL NAME

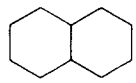
CAS Number: 91-17-8

Chemical Name: Decahydronaphthalene

Synonyms: Decalin
Bicyclo[4,4,0]decane
Naphthane

Molecular Formula: $C_{10}H_{18}$

Structure:



Chemical Properties

Molecular Weight: 138.3

Physical State: Liquid

Vapor Pressure: cis:1 mm at 22.5°C
trans:10 mm at 47.2°C

Vapor Density: 4.76

Boiling Point:

Melting Point: cis:-43.2°C
trans:-31.5°C

Density: cis:0.8927 20°C/4°C
trans:0.8700 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Decahydronaphthalene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	4170 mg/kg	rat	oral
LC_{Lo}	500 ppm (2 hours)	rat	inhalation

Non-lethal Acute Effects:

Irritant–skin, eyes, and mucous membranes

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects: Damage to kidney

Decyl alcohol

CHEMICAL NAME

CAS Number: 112-30-1

Chemical Name: Decyl alcohol

Synonyms: n-Decyl alcohol
1-Decanol
Nonyl carbenol

Molecular Formula: $C_{10}H_{22}O$

Structure: $CH_3 (CH_2)_8 - CH_2 OH$

Chemical Properties

Molecular Weight: 158.3

Physical State: Liquid

Vapor Pressure: 1 mm at 69.5°C

Vapor Density: 5.3

Boiling Point: 232.9°C

Melting Point: 6°C

Density: 0.8297 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Decyl alcohol

PRODUCTION DATA

Annual U.S. Production: 152.5 x 10^6 lbs. (1968)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	4720 mg/kg	rat	oral
LC_{50}	4000 mg/m^3	mouse	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Deet

CHEMICAL NAME

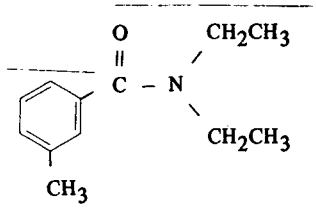
CAS Number: 134-62-3

Chemical Name: N,N-Diethyl-m-toluamide

Synonyms: 3-Methyl-N,N-diethyl benzamide

Molecular Formula: $C_{12}H_{17}NO$

Structure:



Chemical Properties

Molecular Weight: 191.30

Physical State: Liquid

Vapor Pressure: <10 mm at 25°C

Vapor Density:

Boiling Point: 160°C at 19 mm

Melting Point:

Density: 0.996 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 10×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 1.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2000 mg/kg	rat	oral
	200 mg/kg	rat	oral
	3180 mg/kg	rabbit	skin
LD_{Lo}	75 mg/kg	rabbit	intravenous

Non-lethal Acute Effects:

Irritant to eyes and mucous membranes
CNS disturbances

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

DEF

CHEMICAL NAME

CAS Number: 78-48-8

Chemical Name: S,S,S,-Tributyl phosphorotrithioate

Synonyms: S,S,S,-Tributyl trithiophosphate
Butyl phosphorotrithioate

Molecular Formula: $C_{12}H_{27}OPS_3$

Structure: $(CH_3CH_2CH_2CH_2S)_3P = O$

Chemical Properties

Molecular Weight: 314.43

Physical State: Liquid

Vapor Pressure: <10 mm at 25°C

Vapor Density:

Boiling Point: 150°C at 0.3 mm

Melting Point: 25°C

Density:

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 5×10^6 lbs.

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 5.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	150 mg/kg	rat	oral
	168 mg/kg	rat	skin

Non-lethal Acute Effects:

Muscle cramps
Cyanosis
Pulmonary edema
Coma
Convulsion

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:
Cumulative effects

Diacetone alcohol

CHEMICAL NAME

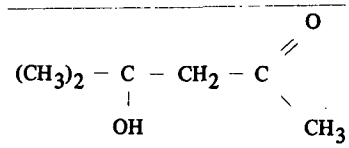
CAS Number: 123-42-2

Chemical Name: 4-Hydroxy-4-methyl-2-pentanone

Synonyms: 4-Hydroxy-2-keto-4-methylpentane
Diacetone alcohol

Molecular Formula: $C_6H_{12}O_2$

Structure:



Chemical Properties

Molecular Weight: 116.2

Physical State: Liquid

Vapor Pressure: 1.1 mm at 20°C

Vapor Density: 4.00

Boiling Point: 167.9°C

Melting Point: -42.8°C

Density: 0.9306 at 25°C/4°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	4000 mg/kg	rat	oral
	93 mg/kg	mouse	intraperitoneal

Non-lethal Acute Effects:

Narcotic in high concentrations
Anemia
Lesions in liver and kidney

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 50 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diaminobenzoic acid

CHEMICAL NAME

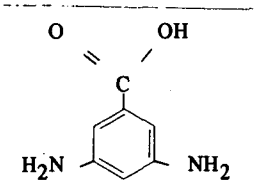
CAS Number: 535-87-5

Chemical Name: 3,5-Diaminobenzoic acid

Synonyms:

Molecular Formula: $C_7H_8N_2O_2$

Structure:



Chemical Properties

Molecular Weight: 152.16

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 240°C

Solubility: Slightly soluble (H_2O)
(Soluble in hot H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Diaminobenzoic acid

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diazinon

CHEMICAL NAME

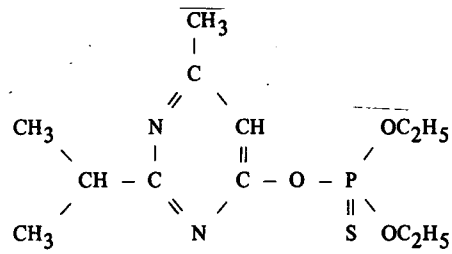
CAS Number: 333-41-5

Chemical Name: Phosphorothioic acid, O,O-diethyl-O-(2-isopropyl-6-methyl-4-pyrimidyl)ester

Synonyms: O,O-Diethyl-O-(2-isopropyl-4-methyl-6-pyrimidinyl)-phosphorothioate

Molecular Formula: $C_{12}H_{21}N_2O_3PS$

Structure:



Chemical Properties

Molecular Weight: 304.38

Physical State: Liquid

Vapor Pressure: 1.4×10^{-4} mm at 20°C

Vapor Density:

Boiling Point: 84°C at .002 mm

Melting Point:

Density: 1.116 at 20°C/4°C

Solubility: 0.004% at room temperature (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 10×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	76 mg/kg	rat	oral
	455 mg/kg	rat	skin
	85 mg/kg	mouse	oral
	2 mg/kg	wild bird	oral
LD_{Lo}	30 mg/kg	rabbit	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: TWA 100 $\mu g/m^3$

Other Chronic Effects:

Diazomethane

CHEMICAL NAME

CAS Number: 334-88-3

Chemical Name: Diazomethane

Synonyms: Azimethylene

Molecular Formula: CH_2N_2

Structure: $H_2C = \overset{(+)}{N} = \overset{(-)}{N}$

Chemical Properties

Molecular Weight: 42.04

Physical State: Gas

Vapor Pressure:

Vapor Density:

Boiling Point: -23°C

Melting Point: -145°C

Density: 1.45

Solubility: Decomposes (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Explosion–severe with alkali metals

PRODUCTION DATA

Annual U.S. Production: No known production

Consumption: Laboratory reagent only

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LC_{Lo}	175 ppm (10 minutes)	cat	inhalation
TC_{Lo}	272 mg/m^3 (2 weeks)	rat	inhalation
TD_{Lo}	467 mg/kg (22 weeks)	mouse	subcutaneous
	54 mg/kg (52 weeks)	mouse	subcutaneous

Non-lethal Acute Effects:

Irritant leads to asthmatic symptoms
Pulmonary edema
Conjunctivitis
Dermatitis

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 0.2 ppm

Carcinogenicity:

TC_{Lo}	272 mg/m^3 (26 weeks)	rat	inhalation
Neoplastic effects:			
TD_{Lo}	467 mg/kg (22 weeks)	mouse	subcutaneous
	54 mg/kg (52 weeks)	mouse	subcutaneous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dibromodifluoromethane

CHEMICAL NAME

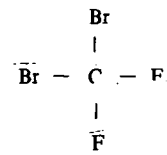
CAS Number: 75-61-6

Chemical Name: Dibromodifluoromethane

Synonyms: Difluorodibromomethane

Molecular Formula: CBr_2F_2

Structure:



Chemical Properties

Molecular Weight:	209.8	**Physical State:**	Heavy liquid
Vapor Pressure:	<10 mm at 25°C	**Vapor Density:**	
Boiling Point:	24.5°C at 760 mm	**Melting Point:**	
Density:	2.288 at 15°C/4°C	**Solubility:**	Soluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–toxic fumes

Dibromodifluoromethane

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LC_{Lo}	2300 ppm	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Di-tert-butyl-p-cresol

CHEMICAL NAME

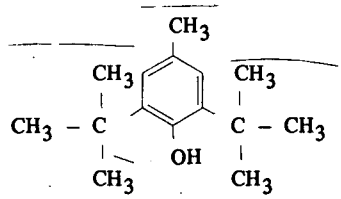
CAS Number: 128-37-0

Chemical Name: 2,6-Di-tert-butyl-p-cresol

Synonyms: DBPC; BHT; Butylated hydroxytoluene
4-Methyl-2,6-di-tert-butylphenol o,o'-Di-tert-butyl-p-cresol

Molecular Formula: $C_{15}H_{24}O$

Structure:



Chemical Properties

Molecular Weight: 220.40

Physical State: Solid

Vapor Pressure: 2.24 mm at 100°C

Vapor Density: 7.6

Boiling Point: 265°C at 760 mm

Melting Point: 71°C

Density: 1.048 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–slight
Disaster hazard–moderate–toxic fumes

Di-tert-butyl-p-cresol

PRODUCTION DATA

Annual U.S. Production: 6.2×10^6 lbs. (1968)
36×10^6 lbs. (1976 capacity)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 18.4 (1972)

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3510 mg/kg	rat	oral
	1040 mg/kg	mouse	oral
LD_{Lo}	250 mg/kg	mouse	intraperitoneal
	940 mg/kg	cat	oral
	2100 mg/kg	rabbit	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TD_{Lo}	550 mg/kg	pregnant rat	oral

TLV:

Other Chronic Effects:

Dibutyl phthalate

CHEMICAL NAME

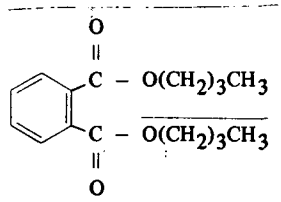
CAS Number: 84-74-2

Chemical Name: Phthalic acid, dibutyl ester

Synonyms: DBP
Dibutylphthalate

Molecular Formula: $C_{16}H_{22}O_4$

Structure:



Chemical Properties

Molecular Weight: 278.33

Physical State: Liquid

Vapor Pressure: 0.01 mm at 20°C

Vapor Density: 9.58

Boiling Point: 340.0°C

Melting Point: -35°C

Density: 1.0484 at 20°C/20°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 19% of theoretical after 5 days at 20°C
Total theoretical oxygen demand = 2.25 (gm/gm)

Atmospheric Reactivity: Reacts with oxidizing agents

Safety Hazard:
Fire–slight

Dibutyl phthalate

PRODUCTION DATA

Annual U.S. Production: 35.5×10^6 lbs. (1974)

Consumption: 35.5×10^6 lbs.

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 29.5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
CNS			
TD_{Lo}	140 mg/kg	human	oral

Chronic Toxicity

U.S. Occupational Standard: TWA 5 mg/m^3

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 5 mg/m^3

TD_{Lo}	874 mg/kg	rat	intraperitoneal

Other Chronic Effects:

2, 4-Dichloroaniline

CHEMICAL NAME

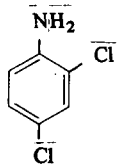
CAS Number: 554-00-7

Chemical Name: 2,4-Dichloroaniline

Synonyms: Dichloroaniline

Molecular Formula: $C_6H_5Cl_2N$

Structure:



Chemical Properties

Molecular Weight: 162.02

Physical State: Solid

Vapor Pressure:

Vapor Density: 5.6

Boiling Point: 245°C at 759mm

Melting Point: 63 to 64°C

Density: 1.567 at 20°C

Solubility: Slightly soluble (H_2O)

Octanol/Water Partition Coefficient: 2.69

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous, toxic fumes

2, 4-Dichloroaniline

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	157 mg/kg	cat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

3, 4-Dichloroaniline

CHEMICAL NAME

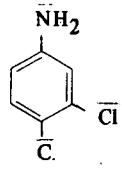
CAS Number: 95-76-1

Chemical Name: 3,4-Dichloroaniline

Synonyms: Dichloroaniline
1-Amino-3, 4-dichlorobenzene

Molecular Formula: $C_6H_5Cl_2N$

Structure:



Chemical Properties

Molecular Weight: 162.02

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 272°C

Melting Point: 72°C

Density:

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

3, 4-Dichloroaniline

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	648 mg/kg	rat	oral
	740 mg/kg	mouse	oral

Non-lethal Acute Effects:

Eye

TC_{Lo}	25 $\mu g/m^3$	human	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

o-Dichlorobenzene

CHEMICAL NAME

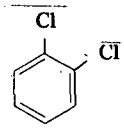
CAS Number: 95-50-1

Chemical Name: o-Dichlorobenzene

Synonyms: DCB
Dichlorobenzol

Molecular Formula: $C_6H_4Cl_2$

Structure:



Chemical Properties

Molecular Weight: 147.0

Physical State: Solid

Vapor Pressure: 1.45 at 25°C

Vapor Density: 5.05

Boiling Point: 180.5°C at 760 mm

Melting Point: −17°C

Density: 1.305 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient: 3.38

Environmental Persistence

BOD:

Atmospheric Reactivity:
Activity toward RO_2: $t_{1/2}$ = 40 days
O_3: $t_{1/2}$ = 1 day
OH: $t_{1/2}$ = 3 days

Safety Hazard:
Fire–moderate

PRODUCTION DATA

Annual U.S. Production: 62.4 x 10^6 lbs.

Consumption: 62.4 x 10^6 lbs.

Fraction of Dispersion: 0.42

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 27.1

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	520 mg/kg	mouse	intravenous
	330 mg/kg	rabbit	intravenous
	2000 mg/kg	guinea pig	oral
LC_{Lo}	707 ppm (7 hours)	rat	inhalation
	800 ppm (24 hours)	guinea pig	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:
- Adenomas
- Carcinomas
- Injection site sarcomas
- Mammary, liver and bladder tumors

Mutagenicity:

Teratogenicity:

TLV: 50 ppm

Other Chronic Effects:
- Respiratory disorders
- Paraplegia and paraparesis
- CNS inhibition
- Kidney hyperplasia

p-Dichlorobenzene

CHEMICAL NAME

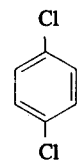
CAS Number: 106-46-7

Chemical Name: p-Dichlorobenzene

Synonyms: DCB
Dichlorobenzol

Molecular Formula: $C_6H_4Cl_2$

Structure:



Chemical Properties

Molecular Weight: 147.0

Physical State: Solid

Vapor Pressure: 10 mm at 54.8°C

Vapor Density:

Boiling Point: 173.4°C at 760 mm

Melting Point: 53°C

Density: 1.2475 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient: 3.39

Environmental Persistence

BOD:

Atmospheric Reactivity:
Activity toward RO_2: $t_{1/2}$ = 40 days
O_3: $t_{1/2}$ = 1 day
OH: $t_{1/2}$ = 3 days

Safety Hazard:
Fire–moderate

p-Dichlorobenzene

PRODUCTION DATA

Annual U.S. Production: 77.3×10^6 lbs.

Consumption: 77.3×10^6 lbs.

Fraction of Dispersion: 0.90

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 70.7

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
P-Dichlorobenzene			
LD_{50}	500 mg/kg	rat	oral
	2500 mg/kg	rat	intraperitoneal
	2950 mg/kg	mouse	oral
LD_{Lo}	2800 mg/kg	guinea pig	oral

Non-lethal Acute Effects:

Unspecified toxic effects			
TD_{Lo}	300 mg/kg	human	oral

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 75 ppm

Carcinogenicity:
- Adenomas
- Carcinomas
- Injection site sarcomas
- Mammary, liver and bladder tumors

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:
- Respiratory disorders
- Paraplegia and paraparesis
- CNS inhibition
- Kidney hyperplasia

Dichlorobenzidine

CHEMICAL NAME

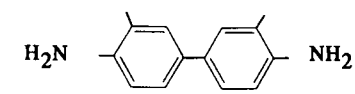
CAS Number: 91-94-1

Chemical Name: 3,3'-Dichlorobenzidine

Synonyms: 4,4'-Diamino-3,3'-dichlorobiphenyl
o,o'-Dichlorobenzidine
3,3'-Dichlorobiphenyl-4,4'diamine

Molecular Formula: $C_{12}H_{10}Cl_2N_2$

Structure:



Chemical Properties

Molecular Weight: 253.02

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point: 133°C

Density:

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 4.6×10^6 lbs.

Consumption:

Fraction of Dispersion: 0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 0.01

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	4740 mg/kg	rat	oral

Non-lethal Acute Effects:

Allergen
Irritant

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

TD_{Lo}	26 gm/kg (50 weeks)	rat	oral
	8 gm/kg (43 weeks)	rat	subcutaneous
	5100 mg/kg (44 weeks)	mouse	oral
	5200 mg/kg (48 weeks)	mouse	subcutaneous
	16 gm/kg	dog	oral
	180 grams (170 weeks)	hamster	oral

Mutagenicity:

Teratogenicity:

TLV: 50 ppm

Other Chronic Effects:

Dichlorodifluoromethane

CHEMICAL NAME

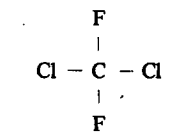
CAS Number: 75-71-8

Chemical Name: Dichlorodifluoromethane

Synonyms: Freon-12

Molecular Formula: CCl_2F_2

Structure:



Chemical Properties

Molecular Weight: 120.92

Physical State: Gas

Vapor Pressure: 5085.93 at 25°C

Vapor Density:

Boiling Point: -29.8°C at 760mm

Melting Point: -158°C

Density: 1.75 at -115°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Activity toward OH: unreactive

Photochemical degradation: non-photo reactive

Possibly reactive toward O_3

Safety Hazard: Disaster–dangerous–toxic fumes of phosgene and fluorides

Dichlorodifluoromethane

PRODUCTION DATA

Annual U.S. Production: 488.4 x 10^6 lbs. (1973)

Consumption: 439.2 x 10^6 lbs.

Fraction of Dispersion: 0.90

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 401.9

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
MLD	324 mg/l	mouse	inhalation

Non-lethal Acute Effects:

Narcotic in high concentrations

Chronic Toxicity

U.S. Occupational Standard: (air) 1000 ppm

Carcinogenicity:

Mutagenicity: May be mutagenic in *N. crassa*

Teratogenicity:

TLV:

Other Chronic Effects: Increase lymphocyte count
Liver damage
Transitory hyperemia

1, 3-Dichloro-5, 5-dimethylhydantoin

CHEMICAL NAME

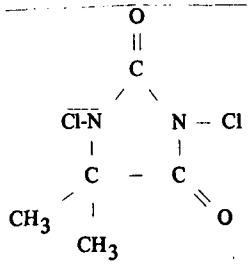
CAS Number: 118-52-5

Chemical Name: 1,3-Dichloro-5,5-dimethyl hydantoin

Synonyms: Dactin
Halane
DDH

Molecular Formula: $C_5H_6Cl_2N_2O_2$

Structure:



Chemical Properties

Molecular Weight: 197

Physical State: Solid

Vapor Pressure: Sublimes at 100°C

Vapor Density: 6.8

Boiling Point:

Melting Point: 130°C

Density: 1.5 at 20°C

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard–dangerous–toxic fumes

1, 3-Dichloro-5, 5-dimethylhydantoin

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	600 mg/kg	rat	oral

Non-lethal Acute Effects:

Irritant to skin
CNS depressant

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 0.2 mg/m^3

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 0.2 mg/m^3

Other Chronic Effects:

Dichloroethylene

CHEMICAL NAME

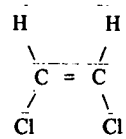
CAS Number: cis: 156-59-2
trans: 156-60-5

Chemical Name: cis: (Z)1,2-Dichloroethylene trans: (E) 1,2-Dichloroethylene

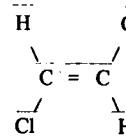
Synonyms: cis-, trans-Dichloroethylene
sym-Dichloroethylene

Molecular Formula:

Structure:



cis



trans

Chemical Properties

Molecular Weight: 96.94

Physical State: Liquid

Vapor Pressure: 204.88 mm at 25°C (mixed isomers)

Vapor Density: 3.34 (mixed isomers)

Boiling Point: 60.3°C at 760 mm (cis)
47.5°C (unspecified pressure) (trans)

Melting Point: −80.5°C (cis)
−50°C (trans)

Density: 1.2837 at 20°C/4°C (cis)
1.2565 at 20°C/4°C (trans)

Solubility: Slightly (H_2O) (cis and trans)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials
Slow decomposition on exposure to air and light

Safety Hazard: Fire–dangerous
Explosion–moderate
Disaster hazard–dangerous–chloride

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
(cis) LD_{50}	770 mg/kg	rat	oral
Central nervous system effects:			
(trans) LD_{Lo}	3,300 mg/m^3	human	inhalation

Non-lethal Acute Effects: (unspecified isomer)

Irritant
Narcotic
Dermatitis
CNS depressant

Chronic Toxicity

U.S. Occupational Standard: (air): TWA 200 ppm (cis)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 200 ppm (cis)

Other Chronic Effects:

Dichloroethyl ether

CHEMICAL NAME

CAS Number: 111-44-4

Chemical Name: Bis(2-chloroethyl) ether

Synonyms: Chlorex
1-Chloro-2-(β-chlorethoxy) ethane
β,β'-Dichloroethyl ether

Molecular Formula: $C_4H_8Cl_2O$

Structure: $Cl\text{-}CH_2CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}Cl$

Chemical Properties

Molecular Weight: 143.0

Physical State: Liquid

Vapor Pressure: 1.23 mm at 25°C

Vapor Density: 4.93

Boiling Point: 178°C at 760 mm

Melting Point: −24.5°C

Density: 1.2199 at 20°C/4°C

Solubility: insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate
Disaster hazard–dangerous–toxic fumes

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	105 mg/kg	rat	oral
	300 mg/kg	guinea pig	skin
LC_{Lo}	1000 mg/kg	rat	inhalation

Non-lethal Acute Effects:

Irritant–eyes and nose, mucous membranes

Chronic Toxicity

U.S. Occupational Standard:
(air) Ceiling level: 15 ppm (skin)

Carcinogenicity:

TD_{Lo}	192 mg/kg (79 weeks)	mouse	oral

Mutagenicity:

Teratogenicity:

TLV: 15 ppm

Other Chronic Effects:

Dichlorofluoromethane

CHEMICAL NAME

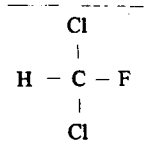
CAS Number: 75-43-4

Chemical Name: Dichlorofluoromethane

Synonyms: Freon 21
Fluorodichloromethane

Molecular Formula: $CHCl_2F$

Structure:



Chemical Properties

Molecular Weight: 103

Physical State: Gas

Vapor Pressure: 1387.5 mm at 25°C

Vapor Density: 3.82

Boiling Point: 8.9°C at 760 mm

Melting Point: -135°C

Density: 1.405 at 9°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard–dangerous–chlorides and fluorides

Dichlorofluoromethane

PRODUCTION DATA

Annual U.S. Production: 487 x 10^6 lbs. (1973)

Consumption: 487 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LC_{Lo}	10,000 ppm (1 hr)	guinea pig	inhalation

Non-lethal Acute Effects:

Narcotic in high concentration

Chronic Toxicity

U.S. Occupational Standard: (air): TWA 1000 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 1000 ppm

Other Chronic Effects:

Dichlorohydrin

CHEMICAL NAME

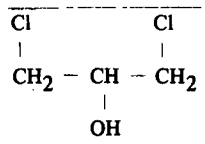
CAS Number: 96-23-1

Chemical Name: 1,3-Dichloro-2-propanol

Synonyms:
- α-Propenyldichlorohydrin
- Glycerol dichlorohydrin
- GDCH
- Dichlorohydrin
- 1,3-Dichloro-2-propanol
- Dichloroisopropyl alcohol

Molecular Formula: $C_3H_6Cl_2O$

Structure:



Chemical Properties

Molecular Weight: 128.99

Physical State: Liquid

Vapor Pressure: 1 mm at 28°C

Vapor Density: 4.45

Boiling Point: 174°C

Melting Point: −4°C

Density: 1.367 at 20°C/4°C

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–moderate
Disaster hazard–dangerous–toxic fumes–phosgene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	490 mg/kg	rat	oral
	800 mg/kg	rabbit	skin
	93 mg/kg	mouse	oral
LC_{Lo}	125 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Irritant–mucous membranes
Anemia
Hepatitis
Nephritis

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dichloropentane

CHEMICAL NAME

CAS Number: 628-76-2

Chemical Name: 1,5-Dichloropentane

Synonyms:

Molecular Formula: $C_5H_{10}Cl_2$

Structure: $Cl - CH_2 - CH_2 - CH_2 - CH_2 - CH_2 - Cl$

Chemical Properties

Molecular Weight: 141.04

Physical State: Liquid

Vapor Pressure: 20 mm at 25°C

Vapor Density: 4.86

Boiling Point: 180°C at 760 mm

Melting Point: -72.8°C

Density: 1.1006 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials
Activity toward O_3: $t_{1/2}$ = 3 days
OH: $t_{1/2}$ = 3 days

Safety Hazard:
Fire–dangerous
Disaster hazard–toxic fumes–phosgene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	64 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

2, 4-Dichlorophenoxyacetic acid

CHEMICAL NAME

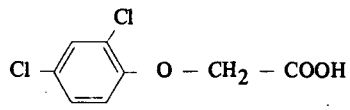
CAS Number: 94-75-7

Chemical Name: (2,4-Dichlorophenoxy) acetic acid

Synonyms: 2,4-D

Molecular Formula: $C_8H_6Cl_2O_3$

Structure:



Chemical Properties

Molecular Weight: 221

Vapor Pressure: 0.4 mm at 160°C

Boiling Point: 160°C at 0.4 mm

Density: 1.560 at 30°C

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density: 7.63

Melting Point: 140 to 141°C

Solubility: Slightly soluble (0.09 gm/100 gm H_2O at 25°C)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard–dangerous–chlorides

2, 4-Dichlorophenoxyacetic acid

PRODUCTION DATA

Annual U.S. Production: 43.0 x 10^6 lbs.

Consumption: 43.0 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 43.4

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	80 mg/kg	human	oral
	375 mg/kg	rat	oral
	1500 mg/kg	rat	skin
	368 mg/kg	mouse	oral
	100 mg/kg	dog	oral
	1400 mg/kg	rabbit	skin
	541 mg /kg	guinea pig	oral
	375 mg/kg	mammal	oral

Non-lethal Acute Effects:

Liver and kidney damage
CNS depressant

Chronic Toxicity

U.S. Occupational Standard: (air): TWA 10 mg/m^3

Carcinogenicity:

Mutagenicity:

Teratogenicity:		TLV:	
TD_{Lo}	25 mg/kg	pregnant rat	oral

Other Chronic Effects:

Dichloropropane

CHEMICAL NAME

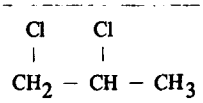
CAS Number: 78-87-5

Chemical Name: 1,2-Dichloropropane

Synonyms: Propylene dichloride

Molecular Formula: $C_3H_6Cl_2$

Structure:



Chemical Properties

Molecular Weight: 113.0

Physical State: Liquid

Vapor Pressure: 53.02 mm at 25°C

Vapor Density: 3.9

Boiling Point: 96.37°C at 760 mm

Melting Point: −100.44°C

Density: 1.1560 at 20°C/4°C

Solubility: Slightly soluble (20 gm/l H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous
Disaster hazard–dangerous–chlorides

PRODUCTION DATA

Annual U.S. Production: 60×10^6 lbs.

Consumption: 60×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.1

Release Rate (million lbs/yr): 60.6

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1900 mg/kg	rat	oral
	860 mg/kg	mouse	oral
LD_{Lo}	5000 mg/kg	dog	oral
LC_{Lo}	2000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Dermatitis

Degeneration of liver, kidney, heart

Chronic Toxicity

U.S. Occupational Standard: (air): TWA 75 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 75 ppm

Other Chronic Effects:

Dichloropropene

CHEMICAL NAME

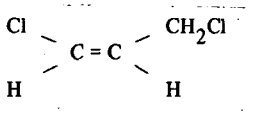
CAS Number: 52-75-6

Chemical Name: 1,3-Dichloropropene

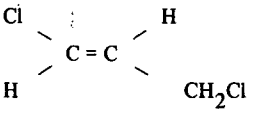
Synonyms: 1,3-Dichloropropylene

Molecular Formula: $C_3H_4Cl_2$

Structure:



Cis



Trans

Chemical Properties

Molecular Weight: 111.0

Physical State: Liquid

Vapor Pressure: 35 mm at 20°C

Vapor Density: 3.8

Boiling Point: 104.3°C (cis)
112°C (trans)

Melting Point:

Density: 1.217 at 20°C/4°C (cis)
1.224 at 20°C/4°C (trans)

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Activity toward RO_2: $t_{1/2}$ = 3 days
Activity toward OH: $t_{1/2}$ = 3 days
From O_3 yields phosgene and chloroacetaldehyde

Safety Hazard: Fire–moderate
Disaster hazard–dangerous–chlorides

PRODUCTION DATA

Annual U.S. Production: 60 x 10^6 lbs.

Consumption: 60 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 60.6

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	250 mg/kg	rat	oral
	200 mg/kg	rabbit	skin
LD_{Lo}	300 mg/kg	mouse	oral
LC_{50}	1000 ppm (4 hours)	man	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Suspected carcinogen

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:
Heart, liver and kidney damage
Highly narcotic

Dichlorotetrafluoroethane

CHEMICAL NAME

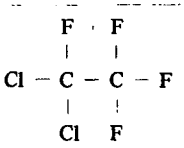
CAS Number: 1320-37-2

Chemical Name: Dichlorotetrafluoroethane

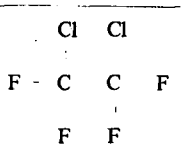
Synonyms: Freon 114
1,1-Dichloro-1,2,2,2-tetrafluoroethane (a)
1,2-Dichloro-1,1,2,2-tetrafluoroethane (b)

Molecular Formula: $C_2Cl_2F_4$

Structure:



(a)



(b)

Chemical Properties (a)

Molecular Weight: 171

Physical State: Gas

Vapor Pressure: 1680.77 mm at 25°C

Vapor Density:

Boiling Point: 3.6°C at 760 mm

Melting Point: -94°C

Density: 1.455 at 25°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Possibly reactive with ozone
Stable in lower atmosphere

Safety Hazard: Disaster hazard–dangerous fluorides and chlorides

Dichlorotetrafluoroethane

PRODUCTION DATA

Annual U.S. Production: 21.7 x 10^6 lbs. (1973)

Consumption: 21.7 x 10^6 lbs.

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Non-lethal Acute Effects:

Narcotic in high concentrations

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 1000 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dicofol

CHEMICAL NAME

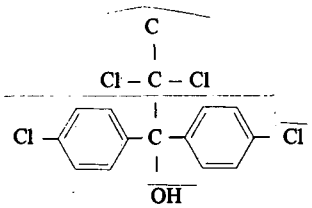
CAS Number: 115-32-2

Chemical Name: 4,4'-Dichloro-α-(trichloromethyl)benzhydrol

Synonyms: 1,1'-Bis(para-chlorophenyl)-2,2,2-trichloroethanol
Dicofol
4,4'-Dichloro-alpha-trichloromethylbenzhydrol

Molecular Formula: $C_{14}H_9Cl_5O$

Structure:



Chemical Properties

Molecular Weight:	370.48	Physical State:	Solid
Vapor Pressure:		Vapor Density:	
Boiling Point:		Melting Point:	77 to 78°C
Density:		Solubility:	
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Temporary environmental (air) contamination

Safety Hazard:

Dicofol

PRODUCTION DATA

Annual U.S. Production: 4.0×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 4.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	575 mg/kg	rat	oral
	100 mg/kg	rat	skin
	1150 mg/kg	rat	intraperitoneal
	1810 mg/kg	rabbit	intraperitoneal
	1870 mg/kg	rabbit	skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dicumyl peroxide

CHEMICAL NAME

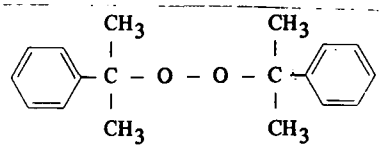
CAS Number: 80-43-3

Chemical Name: Bis(α,α-dimethylbenzyl)peroxide

Synonyms: Cumine peroxide
Isopropylbenzene peroxide
Dicumyl peroxide

Molecular Formula: $C_{18}H_{22}O_2$

Structure:



Chemical Properties

Molecular Weight: 270.40	Physical State: Solid
Vapor Pressure: Negligible	Vapor Density:
Boiling Point:	Melting Point:
Density:	Solubility:
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire—may ignite organic materials on contact

Dicumyl peroxide

PRODUCTION DATA

Annual U.S. Production: 15 x 10^6 lbs.

Consumption: 15 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.02

Release Rate (million lbs/yr): 15.3

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	4100 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

***Teratogenicity*:** **TLV:**

Other Chronic Effects:

Dicyclohexylamine

CHEMICAL NAME

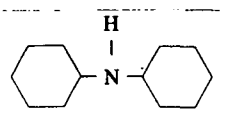
CAS Number: 101-83-7

Chemical Name: Dicyclohexylamine

Synonyms:

Molecular Formula: $C_{12}H_{23}N$

Structure:



Chemical Properties

Molecular Weight: 181.32

Physical State: Liquid

Vapor Pressure: <10 mm at 25°C

Vapor Density: 6.27

Boiling Point: 256°C

Melting Point: -0.10°C

Density: 0.9123 at 20°C/4°C

Solubility: Slightly soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	373 mg/kg	rat	oral
LD_{Lo}	500 mg/kg	mouse	oral

Non-lethal Acute Effects:

Irritant–local irritation and nervous system excitation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplastic effects:

TD_{Lo}	2400 mg/kg (48 week continuous)	mouse	subcutaneous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dieldrin

CHEMICAL NAME

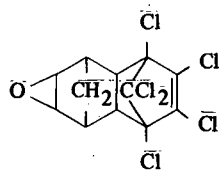
CAS Number: 60-57-1

Chemical Name: 1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-1,4,5,8-dimethanonaphthalene

Synonyms: Compound 497

Molecular Formula: $C_{12}H_8Cl_6O$

Structure:



Chemical Properties

Molecular Weight: 381

Physical State: Solid

Vapor Pressure: 1.78×10^{-7} mm at 20°C

Vapor Density:

Boiling Point:

Melting Point: 176 to 177°C

Density:

Solubility: Insoluble (0.186 mg/l H_2O at 25 to 29°C)

Octanol/Water Partition Coefficient: 4.56

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard—dangerous, toxic fumes, chloride

PRODUCTION DATA

Annual U.S. Production: $<1 \times 10^6$ lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	46 mg/kg	rat	oral
	60 mg/kg	rat (female)	skin
	90 mg/kg	rat (male)	skin
	10.5 mg/kg	mouse	intravenous
	400 mg/kg	rabbit	skin

Non-lethal Acute Effects:

CNS stimulant

27 mg/kg	pigeon	oral
20 mg/kg	chicken	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplastic effects:

TD_{Lo}	730 mg/kg (52 weeks)	mouse	oral
	1800 mg/kg (2 years)	rat	oral

Mutagenicity:

Teratogenicity:

TLV: 100 gm/m^3 (skin)

Other Chronic Effects:

Diethanolamine

CHEMICAL NAME

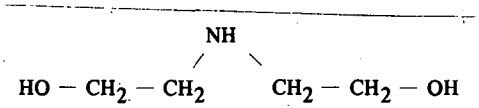
CAS Number: 111-42-2

Chemical Name: 2,2' Iminodiethanol

Synonyms:
DEA
Di (2-hydroxyethyl)-amine
Bis-hydroxyethylamine
Diethylolamine
Diolamine
Diethanolamine

Molecular Formula: $C_4H_{11}NO_2$

Structure:



Chemical Properties

Molecular Weight: 105.14

Physical State: Liquid

Vapor Pressure: 5 mm at 138°C

Vapor Density: 3.65

Boiling Point: 269.1°C

Melting Point: 28.0

Density: 1.0919 at 30°C/20°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient: -2.02

Environmental Persistence

BOD: 88% of total theoretical after 20 days at 20°C

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–slight

Diethanolamine

PRODUCTION DATA

Annual U.S. Production: 101.1 x 10^6 lbs.

Consumption: 86.1 x 10^6 lbs.

Fraction of Dispersion: 0.40

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 36.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	710 mg/kg	rat	oral
	2300 mg/kg	mouse	intraperitoneal
	3553 mg/kg	mouse	subcutaneous

Non-lethal Acute Effects:

Irritation of skin and mucous membranes

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diethylamine

CHEMICAL NAME

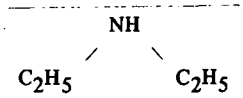
CAS Number: 109-89-7

Chemical Name: Diethylamine

Synonyms: Diethamine

Molecular Formula: $C_4H_{11}N$

Structure:



Chemical Properties

Molecular Weight: 73.1

Physical State: Liquid

Vapor Pressure: 247.1 at 25°C

Vapor Density: 2.53

Boiling Point: 55.5°C

Melting Point: -49.8°C

Density: 0.7108 at 20°C/20°C

Solubility: Very soluble (H_2O)

Octanol/Water Partition Coefficient: 0.82

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous

Diethylamine

PRODUCTION DATA

Annual U.S. Production: 8.8×10^6 lbs. (1970)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	540 mg/kg	rat	oral
	649 mg/kg	mouse	oral
	820 mg/kg	rabbit	skin
LC_{50}	4000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Irritant to skin and mucous membranes
Liver damage

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 25 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 25 ppm

Other Chronic Effects: Extremely dangerous if ingested

Diethylaminoethanol

CHEMICAL NAME

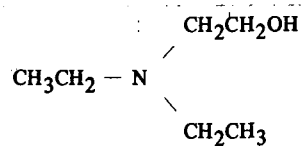
CAS Number: 100-37-8

Chemical Name: 2-(Diethylamino) ethanol

Synonyms: Diethylethanolamine
Diethylaminoethanol

Molecular Formula: $C_6H_{15}NO$

Structure:



Chemical Properties

Molecular Weight: 117.2

Physical State: Liquid

Vapor Pressure: 21 mm at 20°C

Vapor Density: 4.03

Boiling Point: 163°C at 760 mm

Melting Point: -70°C

Density: 0.8921 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient: 0.46

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Diethylaminoethanol

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1300 mg/kg	rat	oral
	1220 mg/kg	rat	intraperitoneal
	1561 mg/kg	mouse	subcutaneous
	1260 mg/kg	rabbit	skin

Non-lethal Acute Effects:

Central nervous system

$\overline{TC}_{Lo}$	200 ppm	human	inhalation

Irritant to skin and mucous membranes

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 10 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 10 ppm

Other Chronic Effects:

Diethylene glycol

CHEMICAL NAME

CAS Number: 111-46-6

Chemical Name: Diethylene glycol

Synonyms: Diglycol
Bis (2-hydroxylethyl) ether
2,2'-Oxydiethanol
Ethylenediglycol
3-Oxa-1,5-pentanediol

Molecular Formula: $C_4H_{10}O_3$

Structure: $HO - CH_2 - CH_2 - O - CH_2 - CH_2 - OH$

Chemical Properties

Molecular Weight: 106.12

Physical State: Liquid

Vapor Pressure: 1 mm at 91.8°C

Vapor Density: 3.66

Boiling Point: 245°C at 760 mm

Melting Point: −10.5°C

Density: 1.1184 at 20°C/20°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient: 1.98

Environmental Persistence

BOD: 67% of theoretical
Total theoretical oxygen demand = 1.5(gm/gm)

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–slight

Diethylene glycol

PRODUCTION DATA

Annual U.S. Production: 350 x 10^6 lbs.

Consumption: 315 x 10^6 lbs.

Fraction of Dispersion: 0.28

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 93.4

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1000 mg/kg	human	oral
	9000 mg/kg	dog	oral
	3300 mg/kg	cat	oral
	2000 mg/kg	rabbit	intravenous

Non-lethal Acute Effects:

Pulmonary edema
Nausea and vomiting
Coma

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diethylene glycol, dibutyl ether

CHEMICAL NAME

CAS Number: 112-73-2

Chemical Name: Bis-(2-butoxyethyl) ether

Synonyms: Bis(α-chloroethyl)ether
Diethylene glycol dibutyl ether

Molecular Formula: $C_{12}H_{26}O_3$

Structure: $C_4H_9 - O - CH_2 - O - C_4H_9$

Chemical Properties

Molecular Weight: 218

Physical State: Liquid

Vapor Pressure: 0.02 mm at 20°C

Vapor Density:

Boiling Point: 256°C

Melting Point: -60.2°C

Density: 0.8853 at 20°C/20°C

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–slight

Diethylene glycol, dibutyl ether

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3900 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diethylene glycol, diethyl ether

CHEMICAL NAME

CAS Number: 112-36-7

Chemical Name: Bis(2-ethoxyethyl) ether

Synonyms: Diethylene glycol diethyl ether

Molecular Formula: $C_8H_{18}O_3$

Structure: $C_2H_5 - O - CH_2 - O - CH_2 - CH_2 - O - C_2H_5$

Chemical Properties

Molecular Weight: 162.26

Physical State: Liquid

Vapor Pressure: <10 mm at 25°C

Vapor Density: 5.6

Boiling Point: 189°C

Melting Point: -44.3°C

Density: 0.9082 at 20°C/20°C

Solubility: Very soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–moderate

Diethylene glycol, diethyl ether

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1850 mg/kg	guinea pig	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diethylene glycol, dimethyl ether

CHEMICAL NAME

CAS Number: 111-96-6

Chemical Name: 1,1'-Oxybis[2-methoxyethane]

Synonyms: Bis(2-methoxyethyl)ether
Dimethylcarbitol
Diglyme

Molecular Formula: $C_6H_{12}O_3$

Structure: $CH_3 - O - CH_2CH_2 - O - CH_2CH_2 - O - CH_3$

Chemical Properties

Molecular Weight:

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 162.0°C

Melting Point: -68.0°C

Density: 0.9451 at 20°C/20°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Diethylene glycol, dimethyl ether

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diethylene glycol, monobutyl ether

CHEMICAL NAME

CAS Number: 18912-80-6

Chemical Name: 2-(2-Isobutoxyethoxy) ethanol

Synonyms:
- Butyl carbitol
- Butoxy diglycol
- O-butyldiethyleneglycol
- Diethylene glycol n-butyl ether
- Diglycol monobutyl ether
- Diethylene glycol monobutyl ether

Molecular Formula: $C_8H_{18}O_3$

Structure: $HO - CH_2 - CH_2 - O - CH_2CH_2 - O - CH_2 - CH_2 - CH_2 - CH_3$

Chemical Properties

Molecular Weight: 162.2

Physical State: Liquid

Vapor Pressure: 0.01 mm at 20°C

Vapor Density: 5.58

Boiling Point: 230.6°C

Melting Point: -68.1°C

Density: 0.9536 at 20°C/20°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Diethylene glycol, monobutyl ether

PRODUCTION DATA

Annual U.S. Production: 41.2×10^6 lbs.

Consumption: 40.2×10^6 lbs.

Fraction of Dispersion: 0.90

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 68.6

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	850 mg/kg	mouse	intraperitoneal
	2000 mg/kg	guinea pig	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diethylene glycol, monobutyl ether acetate

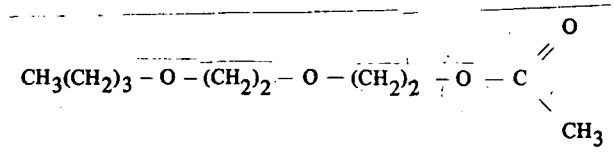
CHEMICAL NAME

CAS Number: 112 – 17 – 4

Chemical Name: Acetic acid, decyl ester

Synonyms: Butyl "carbitol" acetate
Diethylene glycol monobutyl ether acetate

Molecular Formula: $C_{10}H_{20}O_4$

Structure: 

Chemical Properties

Molecular Weight: 204.26

Physical State: Liquid

Vapor Pressure: <0.01 mm at 20°C

Vapor Density:

Boiling Point: 246.7°C at 760 mm

Melting Point: -32.2°C

Density: 0.981 at 20°C/20°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Diethylene glycol, monobutyl ether acetate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2600 mg/kg	rabbit	oral
	2340 mg/kg	guinea pig	oral
	5000 mg/kg	chicken	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diethylene glycol, monethyl ether

CHEMICAL NAME

CAS Number: 111-90-0

Chemical Name: 2-(2-Ethoxyethoxy)ethanol

Synonyms:
- Diethylene glycol monoethylether
- Carbitol
- Diethylene glycol, ethyl ether
- Diglycolmonoethyl ether
- Ethylene diglycol monoethyl ether
- Cellosolve
- Ethoxydiglycol

Molecular Formula: $C_6H_{14}O_3$

Structure: $CH_3CH_2 - O - CH_2CH_2 - O - CH_2CH_2OH$

Chemical Properties

Molecular Weight: 134.17

Physical State: Liquid

Vapor Pressure: <1.0 mm at 20°C

Vapor Density: 4.62

Boiling Point: 201.9°C

Melting Point:

Density: 0.9902 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient: -0.93

Environmental Persistence

BOD: 87% of theoretical after 20 days at 10°C
Total theoretical oxygen demand = 1.9 (gm/gm)

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate

Diethylene glycol, monethyl ether

PRODUCTION DATA

Annual U.S. Production: 24.8×10^6 lbs.

Consumption: 24.8×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 36.8

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2900 mg/kg	rat	intravenous
	5638 mg/kg	mouse	subcutaneous
	3900 mg/kg	mouse	intravenous
	3000 mg/kg	dog	intravenous
	3620 mg/kg	rabbit	oral
	2000 mg/kg	rabbit	subcutaneous
	900 mg/kg	rabbit	subcutaneous
	3070 mg/kg	guinea pig	oral
LD_{Lo}	2000 mg/kg	rat	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diethylene glycol, monoethyl ether acetate

CHEMICAL NAME

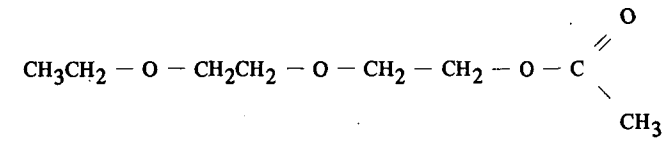
CAS Number: 112-15-2

Chemical Name: 2-(2-Ethoxyethoxy) ethanol acetate

Synonyms: Carbitol acetate
Diethylene glycol monoethyl ether acetate

Molecular Formula: $C_8H_{16}O_4$

Structure:



Chemical Properties

Molecular Weight: 176.21

Physical State: Liquid

Vapor Pressure: 0.05 mm at 20°C

Vapor Density: 6.07

Boiling Point: 217.4°C

Melting Point: -25°C

Density: 1.0114 at 20°C/20°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Diethylene glycol, monoethyl ether acetate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3930 mg/kg	guinea pig	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diethylene glycol, monohexyl ether

CHEMICAL NAME

CAS Number: 112-59-4

Chemical Name: 2-[2-(Hexyloxy)ethoxy] ethanol

Synonyms: Hexyl carbitol
Diethylene glycol monohexyl ether

Molecular Formula: $C_{10}H_{22}O_3$

Structure: $CH_3 - (CH_2)_5 - O - (CH_2) - O - CH_3 - CH_2 - OH$

Chemical Properties

Molecular Weight: 190.32

Physical State: Liquid

Vapor Pressure: 0.01 mm at 20°C

Vapor Density:

Boiling Point: 258.2°C

Melting Point: -33°C

Density: 0.9346 at 20°C/20°C

Solubility:

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–slight

Diethylene glycol, monohexyl ether

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2920 mg/kg	rat	oral
	1500 mg/kg	rabbit	skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diethylene glycol, monomethyl ether

CHEMICAL NAME

CAS Number: 111-77-3

Chemical Name: 2-(2-Methoxyethoxy) ethanol

Synonyms: Methyl carbitol
Diethylene glycol monomethyl ether

Molecular Formula: $C_5H_{12}O_3$

Structure: $CH_3 - O - CH_2 - CH_2 - O - CH_2 - CH_2 - OH$

Chemical Properties

Molecular Weight: 120.15

Physical State: Liquid

Vapor Pressure: 0.2 mm at 20°C

Vapor Density: 4.14

Boiling Point: 194.2°C

Melting Point:

Density: 1.0354 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient: 1.14

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Diethylene glycol, monomethyl ether

PRODUCTION DATA

Annual U.S. Production: 12.7 x 10^6 lbs.

Consumption: 12.7 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 13.1

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	4160 mg/kg	guinea pig	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diethylene glycol, monomethyl ether acetate

CHEMICAL NAME

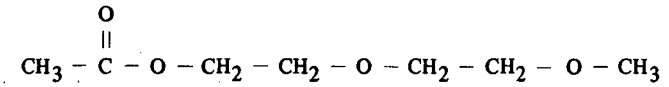
CAS Number: 629-38-9

Chemical Name: 2-(2-Methoxyethoxy)-ethanol, acetate

Synonyms: Methyl carbitol acetate

Molecular Formula: $C_7H_{14}O_4$

Structure:



Chemical Properties

Molecular Weight: 162.19

Physical State: Liquid

Vapor Pressure: 0.12 mm at 20°C

Vapor Density:

Boiling Point: 209.1°C

Melting Point:

Density: 1.0396 at 20°C/20°C

Solubility: Infinite H_2O

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Diethylene glycol, monomethyl ether acetate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3460 mg/kg	guinea pig	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Not tested

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diethylenetriamine

CHEMICAL NAME

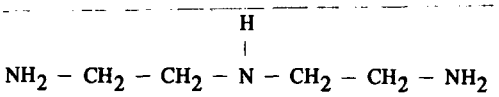
CAS Number: 111-40-4

Chemical Name: 2,2'-Diethylenetriamine

Synonyms: 3-Azapentane-1,5-diamine
Bis [β-aminoethyl] amine
DETA

Molecular Formula: $C_4H_{13}N_3$

Structure:



Chemical Properties

Molecular Weight: 103.17

Physical State: Liquid

Vapor Pressure: 0.22 mm at 20°C

Vapor Density: 3.48

Boiling Point: 207°C at 760 mm

Melting Point: -39°C

Density: 0.9586 at 20°C/20°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 70% of theoretical after 20 days at 20°C

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Diethylenetriamine

PRODUCTION DATA

Annual U.S. Production: 32.4 x 10^6 lbs.

Consumption: 32.4 x 10^6 lbs.

Fraction of Dispersion: 0.50

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 16.7

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1080 mg/kg	rat	oral
	74 mg/kg	rat	intraperitoneal
	71 mg/kg	mouse	intraperitoneal
	1090 mg/kg	rabbit	skin
	1800 mg/kg	guinea pig	skin

Non-lethal Acute Effects:
Irritation of respiratory tract

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: TWA 1 ppm

Other Chronic Effects: Asthma and skin sensitization

Di(2-ethylhexyl) adipate

CHEMICAL NAME

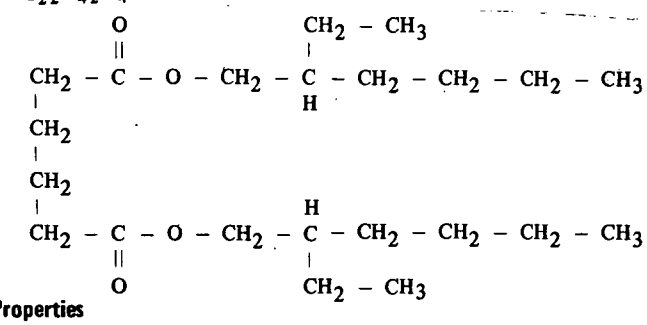
CAS Number: 103-23-1

Chemical Name: Adipic acid, bis (2-ethylhexyl) ester

Synonyms: Bis-(2-ethyl hexyl) adipate
Di-(2-ethylhexyl) adipate
DOA
Dioctyl adipate

Molecular Formula: $C_{22}H_{42}O_4$

Structure:



Chemical Properties

Molecular Weight: 370.58

Physical State: Liquid

Vapor Pressure: <0.01 mm at 20°C

Vapor Density: 12.8

Boiling Point: 214°C at 5 mm

Melting Point: −67.8°C

Density: 0.922 at 25°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Reacts with oxidizing materials
Unreactive towards RO_2 and O_3
Activity toward OH: $t_{1/2}$ = 2.5 days

Safety Hazard: Fire–slight

Di(2-ethylhexyl) adipate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr): 39.4 (1972)

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	900 mg/kg	rat	intravenous
	540 mg/kg	rabbit	intravenous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Negative in rats given 6 gm/kg intraperitoneally in 2 months

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Di(2-ethylhexyl) phthalate

CHEMICAL NAME

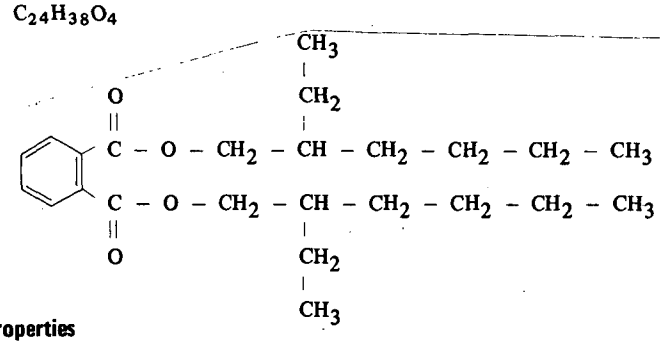
CAS Number: 117-81-7

Chemical Name: Phthalic acid, bis (2-ethylhexyl) ester

Synonyms: Dioctylphthalate
Di-sec-octylphalate
DOP
Di(2-ethylhexyl) phthalate

Molecular Formula: $C_{24}H_{38}O_4$

Structure:



Chemical Properties

Molecular Weight: 390.6

Physical State: Liquid

Vapor Pressure: 1.3 mm at 200°C

Vapor Density: 16.0

Boiling Point: 230°C at 5 mm

Melting Point: -46°C (pour point)

Density: 0.9861 at 20°C/20°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Reacts with oxidizing materials
Unreactive towards RO_2 and O_3
Activity towards OH: $t_{1/2}$ = 1 day

Safety Hazard:
Fire–slight

Di(2-ethylhexyl) phthalate

PRODUCTION DATA

Annual U.S. Production: 389.7 (1974)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Non-lethal Acute Effects:

Gastrointestinal

TD_{Lo}	143 mg/kg	man	oral

Conjunctivitis

Irritant to skin and bronchia

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 5 mg/m^3

Carcinogenicity: Neoplastic effects:

TD_{Lo}	43.2 gm/kg (96 weeks)	rat	oral

Mutagenicity:

TD_{Lo}	15 gm/kg	pregnant rat	intraperitoneal

Teratogenicity: TLV: 5 mg/m^3

TD_{Lo}	30 gm/kg	rat (5-15 days pregnant)	intraperitoneal

Other Chronic Effects:

Embryotoxicity, reduced fetal size, growth retardation, metabolic disturbances, liver enlargement and increased hexobental sleeping time

Diethylstilbestrol

CHEMICAL NAME

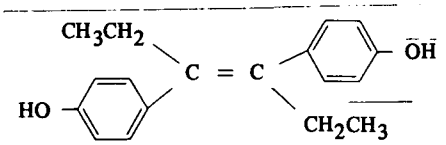
CAS Number: 56-53-1

Chemical Name: α,α'-Diethyl-4,4'-stilbenediol

Synonyms: Stilbesterol
DES
4,4'-(1,2-Diethyl-1,2-ethenediyl)-bis-phenol

Molecular Formula: $C_{18}H_{20}O_2$

Structure:



Chemical Properties

Molecular Weight: 268.3

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 169 to 172°C

Melting Point:

Density:

Solubility: Practically insoluble (H_2O)

Octanol/Water Partition Coefficient: 5.07

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–slight

Diethylstilbestrol

PRODUCTION DATA

Annual U.S. Production: .004 x 10^6 lbs.

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	34 mg/kg	rat	intraperitoneal
	67 mg/kg	mouse	intraperitoneal
LD_{Lo}	2500 mg/kg	mouse	oral

Non-lethal Acute Effects:

Glandular

TD_{Lo}	60 μg/kg (14 days)	human	skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

TD_{Lo}	102 gm/kg (2 years)	rat	oral
	18 mg/kg (368 days)	mouse	oral
	40 mg/kg (40 weeks)	mouse	subcutaneous
	498 mg/kg (44 weeks)	hamster	implant

Cancer in female offspring of women who took diethylstilbesterol during pregnancy

Mutagenicity:

Teratogenicity: **TLV:**

Damage to reproductive tracts of male offspring of women who took diethylstilbesterol during pregnancy

Other Chronic Effects:

Diethyl sulfate

CHEMICAL NAME

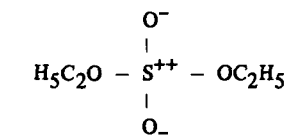
CAS Number: 64-67-5

Chemical Name: Sulfuric acid, diethyl ester

Synonyms: Ethyl
Diethyl sulfate

Molecular Formula: $C_4H_{10}O_4S$

Structure:



Chemical Properties

Molecular Weight: 154.18

Physical State: Liquid

Vapor Pressure: 1 mm at 47°C

Vapor Density: 5.31

Boiling Point: Decomposes to ethyl ether

Melting Point: -24.4°C

Density: 1.1803 at 25°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	350 mg/kg	rat	subcutaneous
	340 mg/kg	rat	intravenous
	647 mg/kg	mouse	oral
LC_{Lo}	250 ppm (4 hours)	rat	inhalation
LD_{Lo}	750 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:				
TD_{Lo}	1900 mg/kg (81 weeks) (intermittent)		rat	oral
(neoplastic)	800 mg/kg (49 weeks) (intermittent)		rat	subcutaneous
Mutagenicity:				
TD_{Lo}	6 mg/kg		mouse	intraperitoneal
Teratogenicity:		TLV:		
TD_{Lo}	85 mg/kg	pregnant	rat	intravenous

Other Chronic Effects:

Difluroethane

CHEMICAL NAME

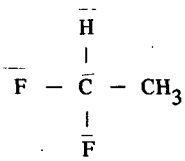
CAS Number: 75-37-6

Chemical Name: 1,1-Difluoroethane

Synonyms: Difluoroethane
Ethylene fluoride
Ethylidene fluoride

Molecular Formula: $C_2H_4F_2$

Structure:



Chemical Properties

Molecular Weight: 66.05

Physical State: Gas

Vapor Pressure: 76 mm at 21°C

Vapor Density: 2.28

Boiling Point: – 24.7

Melting Point: –117°C

Density: 0.95 at 20° (saturated pressure)

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:

Fire–dangerous
Disaster hazard--dangerous–fluorides

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Non-lethal Acute Effects:

Irritant to lungs
Narcotic in high concentrations

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Difolatan

CHEMICAL NAME

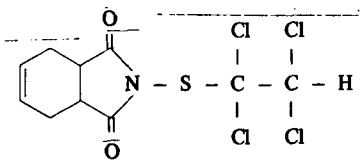
CAS Number: 2425-06-1

Chemical Name: Difolatan

Synonyms: N-(1,1,2,2-tetrachloroethylthio)-4-cyclohexone-1,2-dicarboximide
Ortho 5865

Molecular Formula: $C_{10}H_9Cl_4NO_2S$

Structure:



Chemical Properties

Molecular Weight:	349.06	Physical State:	Solid
Vapor Pressure:		Vapor Density:	
Boiling Point:		Melting Point:	160°C
Density:		Solubility:	Insoluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous chlorides and SO_x

Difolatan

PRODUCTION DATA

Annual U.S. Production: 2 x 10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2500 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: **TLV:**

TD_{Lo}	200 mg/kg	pregnant hamster	oral

Other Chronic Effects:

Reduced weight gain: 2500 ppm (9 weeks)	rat	inhalation

Dihydrotrimethylquinoline

CHEMICAL NAME

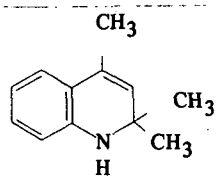
CAS Number: 147-47-7

Chemical Name: 1,2-Dihydro-2,2,4-trimethylquinoline

Synonyms: Acetone anil
Trimethyldihydroquinoline
2,2,4-Trimethyl-1,2,dihydroquinoline
Acetonanil

Molecular Formula: $C_{12}H_{15}N$

Structure:



Chemical Properties

Molecular Weight: 173.3

Physical State: Solid

Vapor Pressure: Negligible at 25°C

Vapor Density:

Boiling Point: Decomposes

Melting Point: 120°C

Density: 1.03 at 25°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–slight

Dihydrotrimethylquinoline

PRODUCTION DATA

Annual U.S. Production: 30.0×10^6 lbs.

Consumption: 26.0×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.30

Release Rate (million lbs/yr): 35.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2000 mg/kg	rat	oral
	1450 mg/kg	mouse	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diisobutylene

CHEMICAL NAME

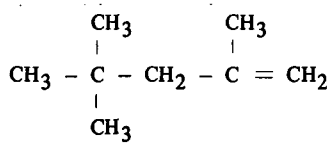
CAS Number: 12002-23-2

Chemical Name: Diisobutylene

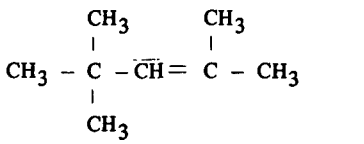
Synonyms: 2,4,4-Trimethyl-1-pentene (a)
2,4,4-Trimethyl-2-pentene (b)

Molecular Formula: C_8H_{16}

Structure:



(a)



(b)

Chemical Properties

Molecular Weight: 112.22

Physical State: Liquid [(a) and (b)]

Vapor Pressure:

Vapor Density: (a) 3.97

Boiling Point: (a) 101.44°C
(b) 104.91°C at 760 mm

Melting Point: (a) -93.48°C
(b) -106.33°C

Density: (a) 0.7150 at 20°C/4°C
(b) 0.7218 at 20°C/4°C

Solubility: Insoluble [(a) and (b)] (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous

Diisobutylene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (*million* lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:
Irritant and narcotic
Liver and kidney damage

Diisobutyl ketone

CHEMICAL NAME

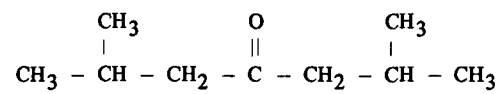
CAS Number: 108-83-8

Chemical Name: 2,6-Dimethyl-4-heptanone

Synonyms: Isovalerone
Diisobutyl ketone

Molecular Formula: $C_9H_{18}O$

Structure:



Chemical Properties

Molecular Weight: 142.2

Physical State: Liquid

Vapor Pressure:

Vapor Density: 4.9

Boiling Point: 168°C at 760 mm

Melting Point:

Density: 0.8053 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire-moderate

Diisobutyl ketone

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LC_{50}	1416 mg/kg	mouse	oral
LC_{Lo}	2000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Irritant
Narcotic in high concentrations

Chronic Toxicity

U.S. Occupational Standard: (air): TWA 25 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diisodecyl phthalate

CHEMICAL NAME

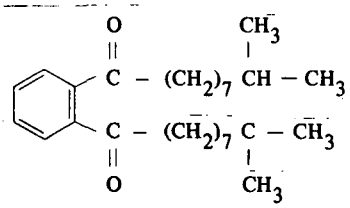
CAS Number: 89-16-7

Chemical Name: 1,2-Benzenedicarboxylic acid, bis(8-methylnonyl)ester

Synonyms: Diisodecyl phthalate
Phthalic acid, bis(8-methylnonyl)ester
DIDP
Plasticizer DDP

Molecular Formula: $C_{28}H_{88}O_4$

Structure:



Chemical Properties

Molecular Weight: 446.7

Physical State: Liquid

Vapor Pressure: <10 mm at 25°C

Vapor Density: 15.4

Boiling Point: 250 to 257°C

Melting Point: -50°C

Density: 0.966 at 25°C/25°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–slight

Diisodecyl phthalate

PRODUCTION DATA

Annual U.S. Production: 153.3 x 10^6 lbs.

Consumption: 133.3 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 135.6

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diisooctyl phthalate

CHEMICAL NAME

CAS Number: 27554-26-3

Chemical Name: 1,2-Benzenedicarboxylic acid, diisooctyl ester

Synonyms: DIOP
Diiso-octyl phthalate
Phthalic acid, diisooctyl ester

Molecular Formula: $C_{24}H_{38}O_4$

Structure:

(C_8H_{17} is predominantly isomeric dimethyl hexanols)

Chemical Properties

Molecular Weight: 390.5

Physical State: Liquid

Vapor Pressure: Negligible at 25°C

Vapor Density: 13.5

Boiling Point: 370°C

Melting Point: −50°C

Density: 0.986 at 20°C/20°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–slight

Diisooctyl phthalate

PRODUCTION DATA

Annual U.S. Production: 43.2 x 10^6 lbs. (1973)

Consumption: 43.2 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): Estimated at 43.2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diisopropylamine

CHEMICAL NAME

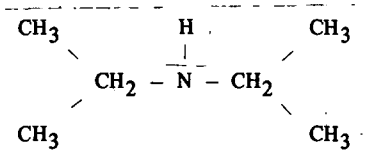
CAS Number: 108-18-9

Chemical Name: Diisopropylamine

Synonyms:

Molecular Formula: $C_6H_{15}N$

Structure:



Chemical Properties

Molecular Weight: 101.19

Physical State: Liquid

Vapor Pressure:

Vapor Density: 3.5

Boiling Point: 84.1°C at 760 mm

Melting Point: −61°C

Density: 0.7169 at 20°C/4°C

Solubility: Slightly soluble (H_2O)

Octanol/Water Partition Coefficient: 1.84

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous

Diisopropylamine

PRODUCTION DATA

Annual U.S. Production: 2×10^6 lbs. (1967)

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	700 mg/kg	rat	oral
LC_{Lo}	1000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Pulmonary edema

Irritant to eyes and respiratory tract

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 5 ppm

Other Chronic Effects:

Diketene

CHEMICAL NAME

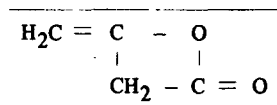
CAS Number: 674-82-8

Chemical Name: 4-Methylene-2-oxetanone

Synonyms: Acetyl ketene
3-Buteno-β-lactone
Diketene

Molecular Formula: $C_4H_4O_2$

Structure:



Chemical Properties

Molecular Weight: 84.07

Physical State: Liquid

Vapor Pressure:

Vapor Density: 2.9

Boiling Point: 127.4°C

Melting Point: -7.5°C

Density: 1.0897

Solubility: Decomposes
Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire--moderate

PRODUCTION DATA

Annual U.S. Production: Dicketene-(none in 1975 in U.S.A.)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	560 mg/kg	rat	oral
LD_{Lo}	800 mg/kg	mouse	oral

Non-lethal Acute Effects:

Irritant to skin and respiratory tract

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dimethoate

CHEMICAL NAME

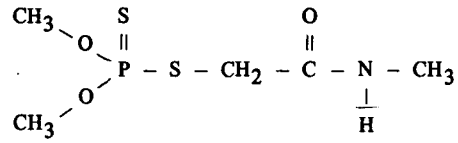
CAS Number: 60-51-5

Chemical Name: Phosphorodithioic acid, S-ester with 2-mercapto-N-methylacetamide O,O-dimethyl ester

Synonyms: O,O-dimethyl S-(N-methylcarbamoylmethyl)phosphorodithioate
Dimethoate

Molecular Formula: $C_5H_{12}NO_3PS_2$

Structure:



Chemical Properties

Molecular Weight: 229.3

Physical State: Solid

Vapor Pressure: 0.025 mm at 25°C

Vapor Density:

Boiling Point: Decomposes

Melting Point: 51 to 52°C

Density:

Solubility: Soluble (H_2O) (1 to 2% at 27°C)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Short-term air contaminant

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 2.0×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	30 mg/kg	human	oral
	147 mg/kg	rat	oral
	353 mg/kg	rat	skin
	250 mg/kg	rat	unknown
	350 mg/kg	guinea pig	oral
	37 mg/kg	chicken	oral
	7 mg/kg	wild bird	oral
LD_{100}	250 mg/kg	rat	oral
	300 mg/kg	cat	oral
	150 mg/kg	mouse	oral

Non-lethal Acute Effects:

Nausea
Lachrymation
Pulmonary edema
Convulsion
Anticholinesterase

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dimethoxybenzidine

CHEMICAL NAME

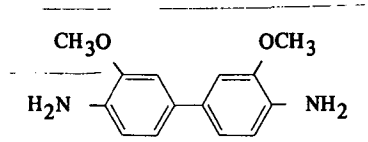
CAS Number: 119-90-4

Chemical Name: 3,3'-Dimethoxybenzidine

Synonyms: O-Dianisidine
Di-para-aminodi-meta-methoxydiphenyl

Molecular Formula: $C_{14}H_{16}N_2O_2$

Structure:



Chemical Properties

Molecular Weight: 244.29

Physical State: Solid

Vapor Pressure:

Vapor Density: 8.5

Boiling Point:

Melting Point: 137 to 138°C

Density:

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–slight

Dimethoxybenzidine

PRODUCTION DATA

Annual U.S. Production: 0.367 x 10^6 lbs. (1967)

Consumption:

Fraction of Dispersion: <0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1920 mg/kg	rat	oral
	3000 mg/kg	dog	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplasms:

TD_{Lo}	13 gm/kg (52 weeks)	rat	oral
	560 gm/kg (70 weeks)	hamster	oral

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

N, N-Dimethylacetamide

CHEMICAL NAME

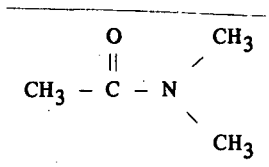
CAS Number: 127-19-5

Chemical Name: N,N-dimethylacetamide

Synonyms: DMAC

Molecular Formula: C_4H_9NO

Structure:



Chemical Properties

Molecular Weight: 87.12

Physical State: Liquid

Vapor Pressure: 1.3 mm at 25°C

Vapor Density: 3.01

Boiling Point: 165°C at 758 mm

Melting Point: -20°C

Density: 0.9366 at 25°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient: -0.77

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–slight

N, N-Dimethylacetamide

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2240 mg/kg	rabbit	skin
Non-lethal Acute Effects:			
Systemic effects TC_{Lo}	20 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 10 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TD_{Lo}	60 mg/kg	**TLV:** pregnant rat	intraperitoneal

Other Chronic Effects:

Dimethylamine

CHEMICAL NAME

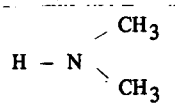
CAS Number: 124-40-3

Chemical Name: Dimethylamine

Synonyms: DMA

Molecular Formula: C_2H_7N

Structure:



Chemical Properties

Molecular Weight: 45.08

Physical State: Gas

Vapor Pressure: 1,290 mm at 25°C

Vapor Density: 1.55

Boiling Point: 7.4°C

Melting Point: −93°C

Density: 0.6804 at 0°C/4°C

Solubility: Very soluble

Octanol/Water Partition Coefficient: −0.38

Environmental Persistence

BOD: Total theoretical oxygen demand 3.5 gm/gm

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:

Fire–dangerous

Explosion–moderate

Dimethylamine

PRODUCTION DATA

Annual U.S. Production: 95.9 x 10^6 lbs.

Consumption: 95.9 x 10^6 lbs.

Fraction of Dispersion: 0.20

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 20.6

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	698 mg/kg	rat	oral
	316 mg/kg	mouse	oral
	240 mg/kg	rabbit	oral
	240 mg/kg	guinea pig	oral

Chronic Toxicity

U.S. Occupational Standard: (air) 10 ppm

Carcinogenicity:

Mutagenicity: Increased incidence of ancuploid cells and structural chromosome changes in rats

Teratogenicity:

TLV: 10 ppm

Other Chronic Effects:

Lung inflammation
Reduced growth rate

Dimethylaminoazobenzene

CHEMICAL NAME

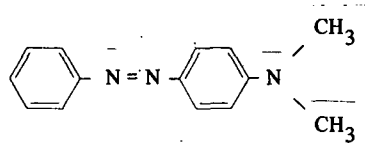
CAS Number: 60-11-7

Chemical Name: C.I. Solvent yellow 2

Synonyms: N,N-Dimethyl-p-phenylazoaniline
p-Dimethylaminoazobenzene
Benzeneazodimethylaniline
Methyl yellow

Molecular Formula: $C_{14}H_{15}N_3$

Structure:



Chemical Properties

Molecular Weight:

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 116°C

Melting Point:

Density:

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	800 mg/kg	rat	oral
	500 mg/kg	rat	intraperitoneal
	300 mg/kg	mouse	oral
	230 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard: (carcinogen)

Carcinogenicity:

Carcinogenic effects:

TD_{Lo}	800 mg/kg (40 days)	rat	oral
	155 mg/kg (4 weeks, intermittent)	rat	skin

Neoplastic effects:

TD_{Lo}	11 gm/kg (12 weeks, continuous)	mouse	oral
	9600 mg/kg (42 weeks, intermittent)	hamster	oral

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dimethylaniline

CHEMICAL NAME

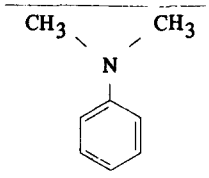
CAS Number: 121-69-7

Chemical Name: N-N-Dimethylaniline

Synonyms: Dimethylaniline

Molecular Formula: $C_8H_{11}N$

Structure:



Chemical Properties

Molecular Weight: 121.18

Physical State: Liquid

Vapor Pressure: 1 mm at 29.5°C

Vapor Density: 4.17

Boiling Point: 193.1°C

Melting Point: 2.5°C

Density: 0.9557 at 20°C/20°C

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient: 2.62

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:

Fire–moderate

Disaster hazard–dangerous–toxic fumes–aniline

PRODUCTION DATA

Annual U.S. Production: 15 x 10^6 lbs. (1967)

Consumption:

***Fraction of* Dispersion:**

***Fraction of* Production Lost:** 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1770 mg/kg	rabbit	skin
LD_{Lo}	50 mg/kg	human	oral
	1410 mg/kg	rat	oral

Non-lethal Acute Effects:

Depressant–CNS

Causes–weakness, tremours, tonic and colonic convulsions, slowness in respiration

Chronic Toxicity

U.S. Occupational Standard: (air) TWA skin 5 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dimethylbutyl acetate

CHEMICAL NAME

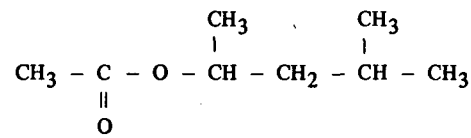
CAS Number: Not listed in 9th Chemical Index

Chemical Name:

Synonyms: Acetic acid, 1,3-dimethylbutyl ester

Molecular Formula: $C_8H_{16}O_2$

Structure:



Chemical Properties

Molecular Weight: 144.24

Physical State:

Vapor Pressure:

Vapor Density: 5.0

Boiling Point: 130 to 137°C

Melting Point:

Density: 0.9

Solubility: Slightly soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–moderate

Dimethylbutyl acetate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (*million lbs/yr*):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LC_{Lo}	4000 ppm	rat	inhalation

Non-lethal Acute Effects:

Eye irritation			
TC_{Lo}	100 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: TWA: 50 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dimethyl ether

CHEMICAL NAME

CAS Number: 115-10-6

Chemical Name: Methyl ether

Synonyms: Methyl oxide
Methoxymethane
Dimethyl ether

Molecular Formula: C_2H_6O

Structure: $CH_3 - O - CH_3$

Chemical Properties

Molecular Weight: 46.07

Physical State: Gas

Vapor Pressure: 551.3 mm at 25°C

Vapor Density: 1.59

Boiling Point: -23.7°C at 760 mm

Melting Point: −138.5°C

Density: 0.661

Solubility: Soluble (74,000 mg/l H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–highly dangerous
Explosion–dangerous

Dimethyl ether

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
Central nervous system depressant			

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

N, N-Dimethylformamide

CHEMICAL NAME

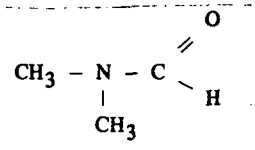
CAS Number: 68-12-2

Chemical Name: N,N-Dimethylformamide

Synonyms: Formic acid, amide

Molecular Formula: C_3H_7NO

Structure:



Chemical Properties

Molecular Weight: 73.11

Physical State: Liquid

Vapor Pressure: 3.7 mm at 25°C

Vapor Density: 2.51

Boiling Point: 152.8°C at 760 mm

Melting Point: −60.48°C

Density: 0.9445 at 25°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

N, N-Dimethylformamide

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	4200 mg/kg	rat	oral
	1260 mg/kg	rat	intraperitoneal
	3500 mg/kg	rat	subcutaneous
	2350 mg/kg	rat	intravenous
	3750 mg/kg	mouse	oral
	650 mg/kg	mouse	intraperitoneal
	470 mg/kg	dog	intravenous
	400 mg/kg	cat	intraperitoneal
	1000 mg/kg	rabbit	intraperitoneal
	1800 mg/kg	rabbit	intravenous
	1030 mg/kg	guinea pig	intravenous

Non-lethal Acute Effects:

Central nervous system

$\overline{TC_{Lo}}$ 20 ppm rat oral

Conjunctivitis

Nausea and vomiting

Anorexia

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 10 ppm (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 10 ppm

Other Chronic Effects: Liver damage

asym-Dimethylhydrazine

CHEMICAL NAME

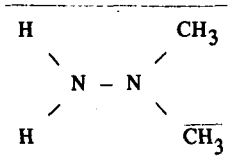
CAS Number: 57-14-7

Chemical Name: 1,1-Dimethylhydrazine

Synonyms: Demazine
Asym-dimethylhydrazine

Molecular Formula: $C_2H_8N_2$

Structure:



Chemical Properties

Molecular Weight: 60.10

Physical State: Liquid

Vapor Pressure: 157 mm at 25°C

Vapor Density: 1.94

Boiling Point: 63.3°C at 752 mm

Melting Point: -58°C

Density: 0.78 at 25°C/4°C

Solubility: Very soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous
Disaster hazard–highly dangerous–toxic fumes

PRODUCTION DATA

Annual U.S. Production: $<1.1 \times 10^6$ lbs.

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	122 mg/kg	rat	oral
	102 mg/kg	rat	intraperitoneal
	265 mg/kg	rat	oral
	125 mg/kg	mouse	oral
	60 mg/kg	mouse	intraperitoneal
	1060 mg/kg	monkey	intraperitoneal
	1329 mg/kg	rabbit	intravenous
LC_{50}	252 ppm (4 hours)	guinea pig	skin
	172 ppm (4 hours)	rat	inhalation
	3578 ppm (15 minutes)	mouse	inhalation
	392 ppm (4 hours)	dog	inhalation

Non-lethal Acute Effects:

Irritant to eyes
Cardiovascular collapse

Chronic Toxicity

U.S. Occupational Standard: TWA: 1 mg/m^3

Carcinogenicity:

TD_{Lo}	7902 mg/kg (30 weeks)	mouse	oral
TD_{Lo}	140 mg/kg (8 weeks)	mouse	intraperitoneal

Mutagenicity:

Teratogenicity:

TLV: 1 mg/m^3

Other Chronic Effects:

sym-Dimethylhydrazine

CHEMICAL NAME

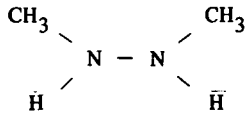
CAS Number: 57-14-7

Chemical Name: 1,2-Dimethylhydrazine

Synonyms: 1,2-Dimethylhydrazine
SDMH

Molecular Formula: $C_2H_8N_2$

Structure:



Chemical Properties

Molecular Weight: 60.11

Physical State:

Vapor Pressure:

Vapor Density:

Boiling Point: 81°C at 753 mm

Melting Point:

Density: 0.8274 at 20°C/4°C

Solubility: Infinitely soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	100 mg/kg	rat	oral
	220 mg/kg	rat	subcutaneous
	95 mg/kg	hamster	intramuscular
LC_{Lo}	280 ppm (4 hours)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

TD_{Lo}	260 mg/kg (13 weeks)	hamster	subcutaneous
	146 mg/kg (31 weeks)	hamster	intramuscular

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

N-(1, 4-Dimethylpentyl)-N'-phenyl-p-phenylenediamine

CHEMICAL NAME

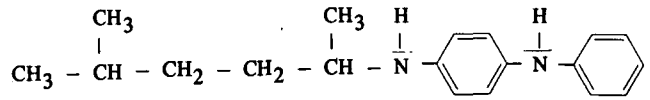
CAS Number: 3081-01-4

Chemical Name: N-(1,4-dimethylpentyl)-N' phenyl-p-phenylenediamine

Synonyms:

Molecular Formula: $C_{19}H_{26}N_2$

Structure:



Chemical Properties

Molecular Weight: 282.24

Physical State: Solid

Vapor Pressure: Negligible at 25°C

Vapor Density:

Boiling Point:

Melting Point: 40 to 44°C

Density:

Solubility:

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Activity toward RO_2: $t_{1/2}$ = 4 days
O_3: $t_{1/2}$ = 1 day
OH: $t_{1/2}$ = 1 day

Safety Hazard:

N-(1, 4-Dimethylpentyl)-N′-phenyl-p-phenylenediamine

PRODUCTION DATA

Annual U.S. Production: 20×10^6 lbs. **Consumption:** 18×10^6 lbs.

Fraction of Dispersion: 0.90 **Fraction of Production Lost:** 0.03

Release Rate (million lbs/yr): 16.8

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: TLV:

Other Chronic Effects:

Dimethylphthalate

CHEMICAL NAME

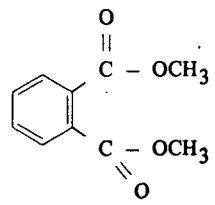
CAS Number: 131-11-3

Chemical Name: Phthalic acid, dimethyl ester

Synonyms: o-Dimethyl phthalate
DMP

Molecular Formula: $C_{10}H_{10}O_4$

Structure:



Chemical Properties

Molecular Weight: 194.18

Physical State: Liquid

Vapor Pressure: 0.01 mm at 20°C

Vapor Density: 6.69

Boiling Point: 283.7°C at 760 mm

Melting Point: 0 to 2°C

Density: 1.1905 at 20.7°C/4°C

Solubility: Very slightly (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Dimethylphthalate

PRODUCTION DATA

Annual U.S. Production: 10.0×10^6 lbs. (1974)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1580 mg/kg	mouse	intraperitoneal
	4400 mg/kg	rabbit	oral
	2400 mg/kg	guinea pig	oral
	8500 mg/kg	chicken	oral
LC_{Lo}	10,000 ppm	cat	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air): TWA 5 mg/m^3

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TD_{Lo}	852 mg/kg	pregnant rat	intraperitoneal

TLV:

Other Chronic Effects:

Dimethyl sulfate

CHEMICAL NAME

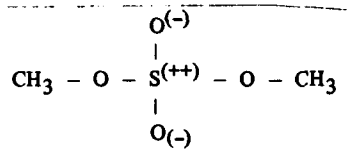
CAS Number: 77-78-1

Chemical Name: Sulfuric acid, dimethyl ester

Synonyms: Dimethyl sulfate
Methyl sulfate

Molecular Formula: $C_2H_6O_4S$

Structure:



Chemical Properties

Molecular Weight: 126.13

Physical State: Liquid

Vapor Pressure:

Vapor Density: 4.35

Boiling Point: 188°C (decomposes)

Melting Point: -26.8°C

Density: 1.3322 at 20°C/4°C

Solubility: Slight (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate
Disaster hazard–dangerous–SO_x

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	440 mg/kg	rat	oral
	100 mg/kg	rat	subcutaneous
	100 mg/kg	rat	intravenous
LD_{Lo}	32 ppm (4 hours)	rat	inhalation
	75 ppm (17 minutes)	mouse	inhalation
	75 ppm (24 minutes)	guinea pig	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

TD_{Lo}:	17 mg/m^3 (18 weeks, intermittent)	rat	inhalation
neoplastic effects			
TD_{Lo}:	200 mg/kg	rat	subcutaneous

Mutagenicity:

Teratogenicity:

		TLV: 1 ppm	
TD_{Lo}:	20 mg/kg	pregnant rat	intravenous

Other Chronic Effects:

Dimethyl sulfide

CHEMICAL NAME

CAS Number: 75-18-3

Chemical Name: Methyl sulfide

Synonyms: Dimethyl sulfide
Methanethiomethane

Molecular Formula: C_2H_6S

Structure: $CH_3 - S - CH_3$

Chemical Properties

Molecular Weight: 62.08

Physical State: Liquid

Vapor Pressure: 530.8 mm at 25°C

Vapor Density: 2.14

Boiling Point: 37.3°C at 760 mm

Melting Point: −98.27°C

Density: 0.8458 at 21°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous
Explosion–moderate
Disaster hazard–dangerous–toxic fumes–SO_x

Dimethyl sulfide

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	535 mg/kg	rat	oral
	3700 mg/kg	mouse	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dimethyl sulfoxide

CHEMICAL NAME

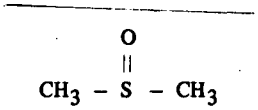
CAS Number: 67-68-5

Chemical Name: Methyl sulfoxide

Synonyms: Dimethyl sulfoxide
DMSO

Molecular Formula: C_2H_6OS

Structure:



Chemical Properties

Molecular Weight: 78.14

Physical State: Liquid (hydroscopic)

Vapor Pressure: 0.37 mm at 20°C

Vapor Density:

Boiling Point: 189°C at 760 mm

Melting Point: 18.45°C

Density: 1.1014 at 20°C/4°C

Solubility: Miscible (H_2O)

Octanol/Water Partition Coefficient: -2.03

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate
Disaster hazard–moderate–toxic fumes

Dimethyl sulfoxide

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	20 mg/kg	rat	oral
	2500 mg/kg	dog	intravenous

Non-lethal Acute Effects:

Allergen
Irritant to skin
Corneal opacity

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

TLV:

Teratogenicity:

TD_{Lo}	5 gm/kg	pregnant rat	oral
	8 gm/kg	pregnant rat	intraperitoneal
	5 gm/kg	mouse	intraperitoneal
	50 mg/kg	hamster	intravenous

Other Chronic Effects:

Dimethyl terephthalate

CHEMICAL NAME

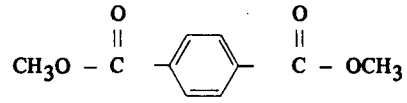
CAS Number: 120-61-6

Chemical Name: Terephthalic acid, dimethyl ester

Synonyms: Dimethylterephthalate
DMT
1,4-Benzene dicarboxylic acid, dimethyl ester
Dimethyl 1,4-benzene carboxylate dimethyl ester

Molecular Formula: $C_{10}H_{10}O_4$

Structure:



Chemical Properties

Molecular Weight: 194.19

Physical State: Solid

Vapor Pressure: 1 mm at 100°C

Vapor Density:

Boiling Point: (sublimes)

Melting Point: 141.0 to 141.8°C

Density: 1.194 at 20°C/4°C

Solubility: Slightly (hot H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Activity toward OH: reactive, estimated half life is 3 days

Safety Hazard:

Dimethyl terephthalate

PRODUCTION DATA

Annual U.S. Production: 2,714 x 10^6 lbs. (1973)

Consumption: 2,714 x 10^6 lbs.

Fraction of Dispersion: 0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 32.5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	4390 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: Negative in rat

TLV:

Other Chronic Effects:

Dinitrobenzenes (m, o, and p)

CHEMICAL NAME

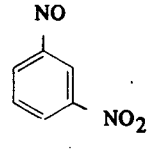
CAS Number: (m): 99-65-0 (o): 528-29-0
(p): 100-25-4

Chemical Name: (o): 1,2-Dinitrobenzene (p): 1,4-Dinitrobenzene
(m): 1,3-Dinitrobenzene

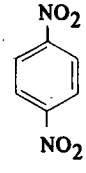
Synonyms: Dinitrobenzol

Molecular Formula: $C_6H_4N_2O_4$

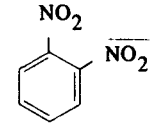
Structure:



(m)



(p)



(o)

Chemical Properties

Molecular Weight: 168.11

Physical State: Solid

Vapor Pressure:

Vapor Density: 5.79 (unspecified isomer)

Boiling Point: (m): 291°C at 756 mm
(p): 299°C at 777 mm
(o): 319°C at 773 mm

Melting Point: (m): 90.02°C
(p): 174°C
(o): 118.5°C

Density: (m): 1.575 at 18°C/4°C
(p): 1.625 at 18°C/4°C
(o): 1.3 119 at 120°C/40°C

Solubility: (m): Slightly (H_2O)
(p) and (o): Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: React with reducing materials

Safety Hazard:
Fire–slight
Explosion–severe
Disaster hazard–dangerous–toxic fumes–NO_x

Dinitrobenzenes (m, o, and p)

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
m-dinitrobenzene			
LD_{50}	42 mg/kg	wild bird species	oral
LD_{10}	27 mg/kg	cat	oral
p-dinitrobenzene			
LD_{10}	29 mg/kg	cat	oral

Non-lethal Acute Effects: (unspecified isomer)
- Anemia
- Jaundice
- Kidney damage
- Injury to CNS

Chronic Toxicity

U.S. Occupational Standard: (air):

m-dinitrobenzene	(air) 1 mg/m^3	skin
p-dinitrobenzene	(air) TWA 1 ppm	skin

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 1 mg/m^3

Other Chronic Effects:

Dinitrobenzoic acid

CHEMICAL NAME

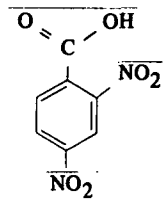
CAS Number: 610-30-0

Chemical Name: 2,4-Dinitrobenzoic acid

Synonyms: Dinitrobenzoic acid

Molecular Formula: $C_7H_4N_2O_6$

Structure:



Chemical Properties

Molecular Weight: 212.12

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point: 183°C

Density:

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dinitro-o-cresol

CHEMICAL NAME

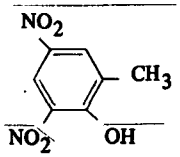
CAS Number: 534-52-1

Chemical Name: 2-Methyl-4,6-dinitrophenol

Synonyms: 4,6-Dinitro-ortho-cresol
DNOC
4,6-Dinitro-2-methyl phenol

Molecular Formula: $C_7H_6N_2O_5$

Structure:



Chemical Properties

Molecular Weight: 198.14

Physical State: Solid

Vapor Pressure: 1.05×10^{-6} mm at 25°C

Vapor Density: 6.82

Boiling Point: 312°C

Melting Point: 85.8°C

Density:

Solubility: Slightly (H_2O) (0.013% at 15°C)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	25 mg/kg	rat	oral
	200 mg/kg	rat	skin
	47 mg/kg	mouse	skin
	19 mg/kg	mouse	intraperitoneal
LC_{Lo}	40 mg/m^3	cat	inhalation

Non-lethal Acute Effects:

Central nervous system			
TC_{Lo}	1 mg/m^3	human	inhalation
Irritant			
Jaundice			
Circulatory collapse			
Mental disorder			

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 200 μg/m^3

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 200 μg/m^3

Other Chronic Effects:

2, 4-Dinitrophenol

CHEMICAL NAME

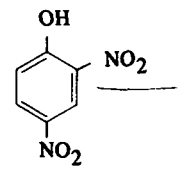
CAS Number: 25550-58-7

Chemical Name: Dinitrophenol

Synonyms: 1-Hydroxy-2,4-dinitrobenzene

Molecular Formula: $C_6H_4N_2O_5$

Structure:



Chemical Properties

Molecular Weight: 184.11

Physical State: Solid

Vapor Pressure:

Vapor Density: 6.35

Boiling Point: Sublimes

Melting Point: 112°C

Density: 1.683 at 24°C

Solubility: 5600 mg/l (H_2O)

Octanol/Water Partition Coefficient: 2.38

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Explosion–moderate

2, 4-Dinitrophenol

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	30 mg/kg	rat	oral
	20 mg/kg	rat	intraperitoneal
	25 mg/kg	rat	subcutaneous
	45 mg/kg	mouse	subcutaneous
	30 mg/kg	rabbit	oral
	81 mg/kg	guinea pig	oral
	13 mg/kg	wild bird	oral

Non-lethal Acute Effects:

Liver damage and kidney damage
Metabolic stimulation
Dermatitis

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects: Cataracts

Dinitrotoluene

CHEMICAL NAME

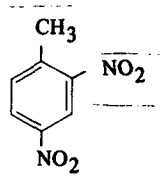
CAS Number: 121-14-2

Chemical Name: 2,4-Dinitrotoluene

Synonyms: Dinitrotoluol
DNT

Molecular Formula: $C_7H_6N_2O_4$

Structure:



Chemical Properties

Molecular Weight: 182.13

Physical State: Solid

Vapor Pressure:

Vapor Density: 6.27

Boiling Point: 300°C (slight decomposition)

Melting Point: 70.5°C

Density: 1.521 at 15°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–moderate
Explosion–moderate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1625 mg/kg	mouse	oral
	268 mg/kg	rat	oral
LD_{Lo}	50 mg/kg	mammal (species unspecified)	subcutaneous

Non-lethal Acute Effects:

Anemia
Liver damage
CNS depression

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 1.5 mg/kg

Other Chronic Effects:

Dinoseb

CHEMICAL NAME

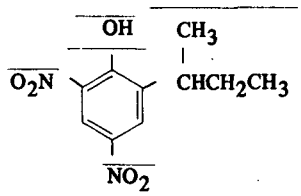
CAS Number: 88-85-7

Chemical Name: 2-(1-Methylpropyl)-4,6-dinitrophenol

Synonyms: 2,4-Dinitro-6-sec-butylphenol
DNBP
Butaphene

Molecular Formula: $C_{10}H_{12}N_2O_5$

Structure:



Chemical Properties

Molecular Weight: 240.2

Physical State: Liquid

Vapor Pressure: 1 mm at 151.1°C

Vapor Density:

Boiling Point: not determined

Melting Point: 32°C

Density: 1.2647 at 45°C

Solubility: Slightly (H_2O) (0.0052 gm/gm at 25°C)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–possible risk

PRODUCTION DATA

Annual U.S. Production: 3.0×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 3.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	25 mg/kg	rat	oral
	80 mg/kg	rat	skin
	20 mg/kg	mouse	oral
	8 mg/kg	mouse	intraperitoneal
	20 mg/kg	guinea pig	oral
	40 mg/kg	chicken	oral
	60 mg/kg	mammal	unknown
	7 mg/kg	wild bird	oral

Non-lethal Acute Effects:

Irritant of eyes and lungs

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

		TLV:	
TD_{Lo}	53 mg/kg	pregnant rat	intraperitoneal

Other Chronic Effects:

Metabolic stimulant

Growth depressant, 0.02% of diet (6 months) rats

Dioxane

CHEMICAL NAME

CAS Number: 123-91-1

Chemical Name: p-Dioxane

Synonyms: 1,4-Dioxane
Para-dioxane
Diethylene ether
Diethylene oxide
Dioxyethylene ether
1,4 Diethylene dioxide

Molecular Formula: $C_4H_8O_3$

Structure:

Chemical Properties

Molecular Weight: 88.1

Physical State: Liquid

Vapor Pressure: 39.7 mm at 25°C

Vapor Density: 3.03

Boiling Point: 101.3°C at 750 mm

Melting Point: 11.8°C

Density: 1.0337 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient: -0.42

Environmental Persistence

BOD:

Atmospheric Reactivity:
Unreactive toward RO_2 and O_3
Activity toward OH: Very reactive $t_{1/2}$ = 9.6 hours

Safety Hazard:
Fire–dangerous
Explosion–moderate

PRODUCTION DATA

Annual U.S. Production: 13.8 x 10^6 lbs.

Consumption: 13.8 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 14.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	790 mg/kg	mouse	intraperitoneal
	2000 mg/kg	cat	oral
	2000 mg/kg	rabbit	oral
	3150 mg/kg	guinea pig	oral
LC_{Lo}	470 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air): TWA 100 ppm skin

Carcinogenicity: TD_{Lo}: 416 gm/kg/57 weeks continuous hepatocarcinomas, kidney carcinomas, carcinomas

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Inhalation causes irritability followed by narcosis, edema and death
Liver and kidney damage
Edema of the brain and lungs

Dioxolane

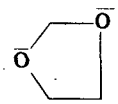
CHEMICAL NAME

CAS Number: 646-06-0

Chemical Name: 1,3-Dioxolane

Synonyms: Dioxolane
Glycol methylene ether

Molecular Formula: $C_3H_6O_2$

Structure: 

Chemical Properties

Molecular Weight: 74.08

Physical State: Liquid

Vapor Pressure: 70 mm at 20°C

Vapor Density: 2.6

Boiling Point: 75°C at 765 mm

Melting Point: −95°C

Density: 1.0600 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3000 mg/kg	rat	oral
	729 mg/kg	mouse	intraperitoneal

Non-lethal Acute Effects:

TD_{Lo}	7 mg/kg	human	oral

Psychotropic effect
Inhalation and ingestion can have moderate effects

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diphenamid

CHEMICAL NAME

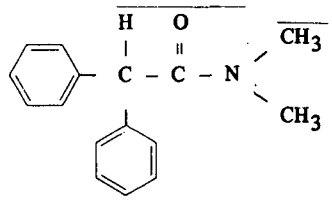
CAS Number: 957-51-7

Chemical Name: N,N-Dimethyl-α-phenylbenzeneacetamide

Synonyms: N,N-Dimethyl-2,2-diphenylacetamide

Molecular Formula: $C_{16}H_{17}NO$

Structure:



Chemical Properties

Molecular Weight: 239.32

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: decomposes at 210°C

Melting Point: 134.5 to 135.5°C

Density: 1.17 at 23.3°C

Solubility: Slightly soluble (H_2O) (0.026 gm/100 ml at 27°C)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Relatively resistant to decomposition by ultraviolet irradiation

Safety Hazard:

Diphenamid

PRODUCTION DATA

Annual U.S. Production: 3.0×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 3.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	293 mg/kg	rat	oral
	600 mg/kg	mouse	oral
	500 mg/kg	mouse	intraperitoneal
	800 mg/kg	mouse	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Emetic

May produce convulsions

Diphenyl

CHEMICAL NAME

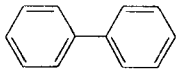
CAS Number: 92-52-4

Chemical Name: Biphenyl

Synonyms: Diphenyl

Molecular Formula: $C_{12}H_{10}$

Structure:



Chemical Properties

Molecular Weight: 154.22

Physical State: Solid

Vapor Pressure: 0.017 psi at 71.1°C

Vapor Density: 5.31

Boiling Point: 255.9°C at 760 mm

Melting Point: 71°C

Density: 0.8660 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient: 4.09

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–slight

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3280 mg/kg	rat	oral
	2400 mg/kg	rabbit	oral
	2500 mg/kg	rabbit	skin

Non-lethal Acute Effects:

Irritant effects

TD_{Lo}	4400 $\mu g/m^3$	human	inhalation

Paralysis and convulsions

Chronic Toxicity

U.S. Occupational Standard: (air): TWA 0.2 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 0.2 ppm

Other Chronic Effects:

Diphenylamine

CHEMICAL NAME

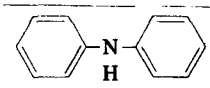
CAS Number: 122-39-4

Chemical Name: Diphenylamine

Synonyms: Phenylaniline
Anilinobenzene
DPA

Molecular Formula: $C_{12}H_{11}N$

Structure:



Chemical Properties

Molecular Weight: 169.24

Physical State: Solid

Vapor Pressure: 1 mm at 108.3°C

Vapor Density: 5.82

Boiling Point: 302°C

Melting Point: 52.85°C

Density: 1.160 at 22°C/20°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient: 3.50

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–slight
Disaster hazard–dangerous–toxic fumes

Diphenylamine

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	3000 mg/kg	rat	oral
	250 mg/kg	mouse	intraperitoneal

Non-lethal Acute Effects:

CNS depression
Cardiac arrhythmia
Liver and kidney damage
Hypertension

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Recognized carcinogen

Mutagenicity:

Teratogenicity:

TLV: 1 mg/m^3

TD_{Lo}:	7500 mg/kg	pregnant rat	oral

Other Chronic Effects:

Diphenyl oxide

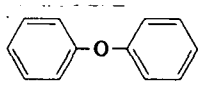
CHEMICAL NAME

CAS Number: 101-84-8

Chemical Name: Phenyl ether

Synonyms: Diphenyl oxide
Diphenyl ether

Molecular Formula: $C_{12}H_{10}O$

Structure: 

Chemical Properties

Molecular Weight: 170.20

Physical State: Liquid

Vapor Pressure: 1 mm at 66°C

Vapor Density: 5.86

Boiling Point: 258°C at 760 mm

Melting Point: 27°C

Density: 1.0728 at 20°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate

Diphenyl oxide

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3370 mg/kg	rat	oral

Non-lethal Acute Effects:
Slight irritant

Chronic Toxicity

U.S. Occupational Standard: (air): TWA 1 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:
Liver, spleen, kidney, thyroid and gastrointestinal system

Diphenylthiourea

CHEMICAL NAME

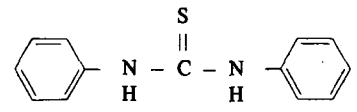
CAS Number: 102-08-9

Chemical Name: Thiocarbanilide

Synonyms: Diphenylthiourea
N,N-Diphenylthiourea
1,3-Diphenyl-2-thiourea

Molecular Formula: $C_{13}H_{12}N_2S$

Structure:



Chemical Properties

Molecular Weight: 228.33

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: Decomposes

Melting Point: 148°C

Density: 1.32 at 25°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–toxic fumes–SO_x

Diphenylthiourea

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	500 mg/kg	mouse	intraperitoneal
LD_{Lo}	720 mg/kg	cat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dipropylene glycol

CHEMICAL NAME

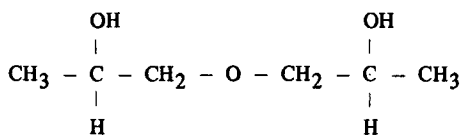
CAS Number: 106-62-7

Chemical Name: Dipropylene glycol

Synonyms: 2,2'-Dihydroxy dipropyl ether

Molecular Formula: $C_6H_{14}O_3$

Structure:



Chemical Properties

Molecular Weight: 134.17

Physical State: Liquid

Vapor Pressure: 0.01 mm at 20°C

Vapor Density: 4.63

Boiling Point: 231.8°C

Melting Point:

Density: 1.0252 at 20°C/20°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient: -1.23

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–slight

Dipropylene glycol

PRODUCTION DATA

Annual U.S. Production: 67 x 10^6 lbs. (1976 capacity)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
None listed (Moderate)			

Non-lethal Acute Effects:
Moderate effects

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dipropylene glycol, monomethyl ether

CHEMICAL NAME

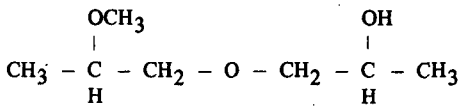
CAS Number: 20324-32-7

Chemical Name: Dipropylene glycol monomethyl ether

Synonyms: Dowanol 50B

Molecular Formula: $C_7H_{16}O_3$

Structure:



Chemical Properties

Molecular Weight: 148.20

Physical State: Liquid

Vapor Pressure: Negligible

Vapor Density: 5.11

Boiling Point: 189°C

Melting Point: -80°C

Density: 0.950 at 25°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Dipropylene glycol, monomethyl ether

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	7500 mg/kg	dog	oral
LD_{Lo}	4900 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard: (air): TWA 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Disodium methanearsonate

CHEMICAL NAME

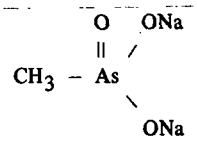
CAS Number: 144-21-8

Chemical Name: Methanearsonic acid, disodium salt

Synonyms: DMA
Disodium methanearsonate
Crab-e-rad
Arsinyl
DSMA

Molecular Formula: $CH_3AsO_3 \cdot 2Na$

Structure:



Chemical Properties

Molecular Weight: 183.94

Physical State: Solid

Vapor Pressure: Very low

Vapor Density:

Boiling Point:

Melting Point: 132 to 139°C

Density: ca. 1.0

Solubility: Very soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Disodium methanearsonate

PRODUCTION DATA

Annual U.S. Production: 35.0×10^6 lbs.

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1800 mg/kg	rat	oral
	600 mg/kg	mouse	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Disulfoton

CHEMICAL NAME

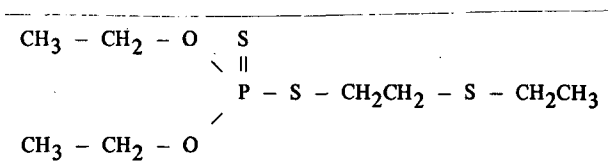
CAS Number: 298-04-4

Chemical Name: Phosphorodithioic O,O-diethyl S-[2-(ethylthio)ethyl] ester

Synonyms: Di-Syston

Molecular Formula: $C_8H_{19}O_2PS_3$

Structure:



Chemical Properties

Molecular Weight: 274

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 62°C at 0.001 mm

Melting Point:

Density: 1.144 at 20°C/4°C

Solubility: Very slightly (H_2O) (1:40,000)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 8.0×10^6 lbs.

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 8.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	6 mg/kg	rat	skin
	5400 μg/kg	rat	intraperitoneal
	2500 μg/kg	rat	unknown
	7 mg/kg	mouse	intraperitoneal
	3.2 mg/kg	wild bird	oral
	12.5 mg/kg	male rat	oral
	2.6 mg/kg	female rat	oral
	20. mg/kg	male rat	dermal

Chronic Toxicity

U.S. Occupational Standard: (air) TWA $\mu g/m^3$

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Chronic oral: 10 ppm (16 weeks) reduced cholinesterase in rat

Ditridecylphthalate

CHEMICAL NAME

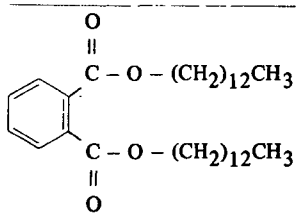
CAS Number: 119-06-2

Chemical Name: Phthalic acid, ditridecyl ester

Synonyms: Ditridecylphthalate
DTDP

Molecular Formula: $C_{34}H_{58}O_4$

Structure:



Chemical Properties

Molecular Weight: 538

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: >285°C at 5 mm

Melting Point: -37°C (pour point)

Density: 0.951 at 20°C/20°C

Solubility:

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–slight

Ditridecylphthalate

PRODUCTION DATA

Annual U.S. Production: 27.2×10^6 lbs. (1974)

Consumption: 27.2×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 24.3 (1972)

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Diuron

CHEMICAL NAME

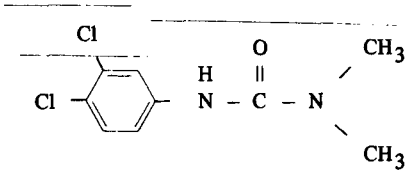
CAS Number: 330-54-1

Chemical Name: 3-(3,4-Dichlorophenyl)-1,1-dimethylurea

Synonyms:

Molecular Formula: $C_9H_{10}Cl_2N_2O$

Structure:



Chemical Properties

Molecular Weight: 233.11

Physical State: Solid

Vapor Pressure: 2×10^{-7} mm at 30°C

Vapor Density:

Boiling Point: 180°C (decomposes)

Melting Point: 153 to 155°C

Density:

Solubility: 42 ppm at 25°C in distilled water

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Photodecomposition insignificant

Safety Hazard:
Disaster hazard–dangerous–toxic fumes

PRODUCTION DATA

Annual U.S. Production: 6.0×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 6.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	437 mg/kg	rat	oral
	3400 mg/kg	rat	oral
LD_{Lo}	500 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Irritant to eyes, nose, throat, and skin

Dodecane

CHEMICAL NAME

CAS Number: 112-40-3

Chemical Name: Dodecane

Synonyms: Bihexyl
Dihexyl

Molecular Formula: $C_{12}H_{26}$

Structure: $CH_3(CH_2)_{10}CH_3$

Chemical Properties

Molecular Weight: 170.3	Physical State: Liquid
Vapor Pressure: 1 mm at 478°C	Vapor Density: 5.96
Boiling Point: 213°C at 760 mm	Melting Point: -10°C
Density: 0.749 at 20°C/4°C	Solubility: Insoluble (H_2O)
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–moderate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dodecylbenzene

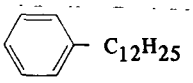
CHEMICAL NAME

CAS Number: 25265-78-5

Chemical Name: Dodecyl benzene

Synonyms: Alkane
Detergent alkylate

Molecular Formula: $C_{18}H_{30}$

Structure: 

Chemical Properties

Molecular Weight: 246.48

Physical State: Liquid

Vapor Pressure: <10 mm at 75°C

Vapor Density: 8.47

Boiling Point: 290°C

Melting Point:

Density: 0.9

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–slight

Dodecylbenzene

PRODUCTION DATA

Annual U.S. Production: 523.3 x 10^6 lbs. (1975)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dodecylbenzenesulfonic acid, sodium salt

CHEMICAL NAME

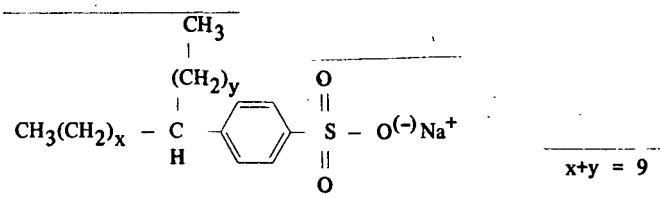
CAS Number: 12068-21-2

Chemical Name: Dodecylbenzenesulfonic acid, sodium salt

Synonyms: Sodium linear alkylatesulfonate (C_{12})
Sodium laurylbenzenesulfonic acid

Molecular Formula: $C_{18}H_{30}O_3S$

Structure:



x+y = 9

Chemical Properties

Molecular Weight: 349.54

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point:

Density:

Solubility: Soluble (400 gm/l H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Unreactive toward RO_2

Safety Hazard:

Dodecylbenzenesulfonic acid, sodium salt

PRODUCTION DATA

Annual U.S. Production: 364.1 x 10^6 lbs.

Consumption: 364.1 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 369.5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1260 mg/kg	rat	oral
	2000 mg/kg	mouse	oral
	105 mg/kg	mouse	intravenous

Non-lethal Acute Effects:

Skin and mucous membrane irritation
Increased sensitivity to glucose loads
Increased liver weight and fasting sugar level
Decreased growth rate and food consumption

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Negative in rat & mouse

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dodecyl mercaptan

CHEMICAL NAME

CAS Number: 112-55-0

Chemical Name: 1-Dodecanethiol

Synonyms: DDM
Lauryl mercaptan
N-dodecyl mercaptan
Lauryl mercaptide
N-Dodecyl mercaptan

Molecular Formula: $C_{12}H_{26}S$

Structure: $CH_3(CH_2)_{10}CH_2SH$

Chemical Properties

Molecular Weight: 202.4

Physical State: Liquid

Vapor Pressure: Negligible

Vapor Density: 6.98

Boiling Point: 142 to 145°C at 15 mm

Melting Point: -7.5°C

Density: 0.845 at 20°C/20°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate
Disaster hazard–dangerous–sulfates

Dodecyl mercaptan

PRODUCTION DATA

Annual U.S. Production: 15×10^6 lbs.

Consumption: 15.2×10^6 lbs.

Fraction of Dispersion: 0.98

Fraction of Production Lost: 0.02

Release Rate (million lbs/yr): 15.2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	309 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dodecylphenol

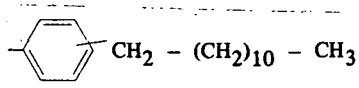
CHEMICAL NAME

CAS Number: 1331-57-3

Chemical Name: Dodecylphenol

Synonyms: Mixture of dodecylphenol isomers

Molecular Formula: $C_{18}H_{30}O$

Structure: 

Chemical Properties

Molecular Weight: 262.4

Physical State: Liquid

Vapor Pressure: <10 mm at 25°C

Vapor Density: 9.04

Boiling Point: 154 to 168°C

Melting Point:

Density: 0.94 at 20°C/20°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Disaster hazard–moderate–toxic fumes

Dodecylphenol

PRODUCTION DATA

Annual U.S. Production: 17.4×10^6 lbs.

Consumption: 17.4×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 17.9

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2140 mg/kg	rat	oral
	5000 mg/kg	rabbit	skin

Non-lethal Acute Effects:
Strong irritant

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dodecyl sulfate, sodium salt

CHEMICAL NAME

CAS Number: 151-21-3

Chemical Name: Sulfuric acid monododecyl ester sodium salt

Synonyms: Dodecyl sulfate, sodium salt
Lauryl sodium sulfate
SDS
Sodium dodecyl sulfate
Sodium lauryl sulfate

Molecular Formula: $C_{12}H_{25}O_4S \cdot Na$

Structure: $CH_3(CH_2)_{10}CH_2 - OSO_3 \cdot Na$

Chemical Properties

Molecular Weight: 289.44

Physical State: Solid

Vapor Pressure: Negligible

Vapor Density:

Boiling Point:

Melting Point:

Density:

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient: 1.60

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Dodecyl sulfate, sodium salt

PRODUCTION DATA

Annual U.S. Production: 26.8 x 10^6 lbs.

Consumption: 26.8 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 27.6

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1300 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dodecyl sulfate, triethanolamine salt

CHEMICAL NAME

CAS Number: 139-96-8

Chemical Name: Sulfuric acid, monododecyl ester, compd. with 2,2',2''-nitrilotris[ethanol] (1:1)

Synonyms: Triethanolamine lauryl sulfate

Molecular Formula: $C_{18}H_{41}NO_7S$

Structure: $CH_3(CH_2)_{10}CH_2 - O - SO_3^{(-)}\ \overset{(+)}{\underset{H}{N}} - (CH_2CH_2OH)_3$

Chemical Properties

Molecular Weight:	415.59	Physical State:	Liquid or paste
Vapor Pressure:		Vapor Density:	
Boiling Point:		Melting Point:	
Density:		Solubility:	
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Dodecyl sulfate, triethanolamine salt

PRODUCTION DATA

Annual U.S. Production: 16.1×10^6 lbs.

Consumption: 16.1×10^6 lbs.

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 16.5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: TLV:

Other Chronic Effects:

Dursban

CHEMICAL NAME

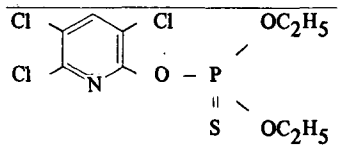
CAS Number: 2921-88-2

Chemical Name: Phosphorodithioic acid, O,O-diethyl-O-(3,5,6-trichloro-2-pyridinyl)ester

Synonyms: O,O-Diethyl-O-(3,5,6-trichloro-2-pyridyl)phosphorothioate

Molecular Formula: $C_9H_{11}Cl_3NO_3PS$

Structure:



Chemical Properties

Molecular Weight: 349.5

Physical State: Solid

Vapor Pressure: 1.87×10^{-5} mm

Vapor Density:

Boiling Point:

Melting Point: 41 to 43°C

Density:

Solubility: Very slightly (H_2O) (0.0002 gm/100 ml)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Disaster hazard—dangerous—chlorides, parathion

PRODUCTION DATA

Annual U.S. Production: 5.0×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 5.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	145 mg/kg	rat	oral
	202 mg/kg	rat	skin
	150 mg/kg	rat	unreported
	2000 mg/kg	rabbit	skin
	500 mg/kg	guinea pig	unreported
	27 mg/kg	pigeon	oral
	24 mg/kg	chicken	oral
	16 mg/kg	quail	oral
	76 mg/kg	duck	oral
	8 mg/kg	wild bird	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Dyfonate

CHEMICAL NAME

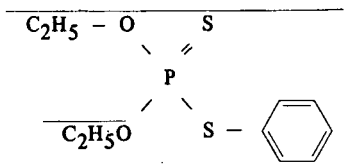
CAS Number: 944-22-9

Chemical Name: Ethylphosphonodithioic acid, O-ethyl,S-phenyl ester

Synonyms: O-Ethyl-S-phenylethylphosphodithioate

Molecular Formula: $C_{10}H_{15}OPS_2$

Structure:



Chemical Properties

Molecular Weight:	246.34	Physical State:	Liquid
Vapor Pressure:		Vapor Density:	
Boiling Point:		Melting Point:	100°C at 0.3 mm Hg.
Density:		Solubility:	
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Disaster hazard–dangerous–phosphates

Dyfonate

PRODUCTION DATA

Annual U.S. Production: 2.0×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3 mg/kg	rat	oral
	147 mg/kg	rat	skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Endosulfan

CHEMICAL NAME

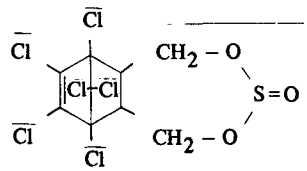
CAS Number: 115-29-7

Chemical Name: 1,4,5,6,7,7-Hexachloro-5-norbornene-2,3-dimethanol,cyclic sulfite

Synonyms: Thiodan
6,7,8,9,10,10-Hexachloro-1,5,5a,6,9,9a-hexahydro-6,9-methano-2,3,4-benzo (e)-dioxathiepin-3-oxide

Molecular Formula: $C_9H_6Cl_6O_3S$

Structure:



Chemical Properties

Molecular Weight: 406.91

Physical State: Solid

Vapor Pressure: (no measurable pressure at 75°C)

Vapor Density:

Boiling Point:

Melting Point: 106°C

Density: 1.745 at 20°C/20°C

Solubility: Nearly insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 2.0 x 10^6 lbs.

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	18 mg/kg	rat	oral
	74 mg/kg	rat	skin
	40 mg/kg	rat	unreported
	359 mg/kg	rabbit	skin
	34 mg/kg	duck	oral
	35 mg/kg	wild bird	oral

affects central nervous system

Chronic Toxicity

U.S. Occupational Standard: (air) TWA: 100 $\mu g/m^3$ (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Endothal

CHEMICAL NAME

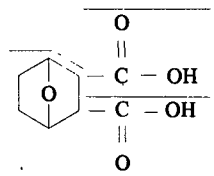
CAS Number: 145-73-3

Chemical Name: 7-Oxabicyclo(2.2.1)heptane-2,3-dicarboxylic acid

Synonyms: 3,6-Endohexanhydrophthalic acid

Molecular Formula: $C_8H_{10}O_5$

Structure:



Chemical Properties

Molecular Weight: 232.16

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: Slowly decomposes above 90°C

Melting Point: ca. 144°C when heated rapidly (decomposes)

Density: 1.431

Solubility: Soluble (10 gm/100 gm H_2O at 20°C)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 2.0×10^6 lbs.

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
$2D_{50}$	38 to 51 mg/kg	rat	oral
LD_{50}	51 mg/kg	rat	oral
	750 mg/kg	rat	skin
	100 mg/kg	rabbit	skin
LD_{Lo}	50 mg/kg	mouse	oral
	5 mg/kg	dog	intravenous
	200 mg/kg	rabbit	oral
	5 mg/kg	rabbit	intravenous
	250 mg/kg	guinea pig	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Irritant to skin, nose, eyes, and throat
Greatest occupational hazard-eye irritation by burning of exposed tissues

Epichlorohydrin

CHEMICAL NAME

CAS Number: 106-89-8

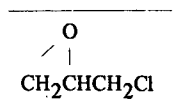
Chemical Name: 1-Chloro-2,3-epoxypropane

Synonyms: α: 3-Chloro-1,2-propylene

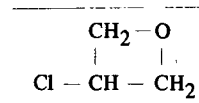
β : 3-Chloro-1-oxacyclobutane
3-Chlorooxetane

Molecular Formula: C_3H_5ClO

Structure:



α



β

Chemical Properties (α)

Molecular Weight: 92.53

Physical State: Liquid

Vapor Pressure: 16.8 mm at 25°C

Vapor Density: 3.29

Boiling Point: 117.9°C

Melting Point: -48°C

Density: 1.1801 at 20°C/4°C

Solubility: Slightly soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate
Disaster hazard–dangerous, toxic fumes–phosgene

Epichlorohydrin

PRODUCTION DATA

Annual U.S. Production: 495 x 10^6 lbs. (1974)

Consumption: ca. 396 x 10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	90 mg/kg	rat	oral
	238 mg/kg	mouse	oral
	155 mg/kg	mouse	intraperitoneal
LC_{50}	100 mg/kg	rabbit	skin
LC_{Lo}	250 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Eye effects:

TD_{Lo}	20 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard:
TWA : 5 ppm

Carcinogenicity:

Neoplastic effects:

TD_{Lo}	19 mg/kg	mouse	inhalation
	720 mg/kg	mouse	subcutaneous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Eptam

CHEMICAL NAME

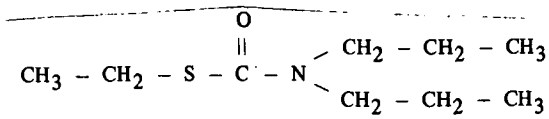
CAS Number: 759-94-4

Chemical Name: S-Ethyldipropylthiocarbamate

Synonyms: Dipropylthiocarbamic acid, S-ethyl ester
S-Ethyl-N,N-propylthiocarbamate

Molecular Formula: $C_9H_{19}NOS$

Structure:



Chemical Properties

Molecular Weight: 189.35

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 232°C at 760 mm

Melting Point:

Density: 0.9546 at 30°C

Solubility: Very slightly soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 5 x 10^6 lbs.

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 5.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1630 mg/kg	rat	oral
	750 mg/kg	mouse	oral
	112 mg/kg	cat	oral
	146 mg/kg	rabbit	skin
	100 mg/kg	wild bird	oral
LC_{Lo}	200 mg/m^3/(3 hours)	rat	inhalation
	400 mg/m^3/(3 hours)	cat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Neoplastic

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethane

CHEMICAL NAME

CAS Number: 74-84-0

Chemical Name: Ethane

Synonyms: Bimethyl
Dimethyl
Ethyl hydride
Me Me
Methylmethane

Molecular Formula: C_2H_6

Structure: $CH_3 - CH_3$

Chemical Properties

Molecular Weight: 30.07

Physical State: Gas

Vapor Pressure: 255 mm at 21°C

Vapor Density: 1.04

Boiling Point: -88.63°C

Melting Point: -183.3°C

Density: 0.446 at 0°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–dangerous
Explosion–moderate

Ethane

PRODUCTION DATA

Annual U.S. Production: 5,485 x 10^6 lbs. (1973)

Consumption: 5,485 x 10^6 lbs.

Fraction of Dispersion: 0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 54.9

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethanolamine

CHEMICAL NAME

CAS Number: 141-43-5

Chemical Name: 2-Aminoethanol

Synonyms: 2-Aminoethanol
Monoethanolamine
β-Ethanolamine
Colamine

Molecular Formula: C_2H_7NO

Structure: $H_2N - CH_2 - CH_2 - OH$

Chemical Properties

Molecular Weight: 61.08

Physical State: Liquid

Vapor Pressure: 6 mm at 60°C

Vapor Density: 2.11

Boiling Point: 170°C at 760 mm

Melting Point: 10.3°C

Density: 1.0180 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient: 1.71

Environmental Persistence

BOD: 75% of theoretical after 30 days at 20°C at 25 mg/ml
Total theoretical oxygen demand = 2.62 (gm/gm)

Atmospheric Reactivity:
Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Ethanolamine

PRODUCTION DATA

Annual U.S. Production: 293 x 10^6 lbs. (1973)

Consumption: 266 x 10^6 lbs. (1974)

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2100 mg/kg	rat	oral
	981 mg/kg	rat	intraperitoneal
	2537 mg/kg	mouse	subcutaneous

Chronic Toxicity

U.S. Occupational Standard: (air) TWA: 3 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethion

CHEMICAL NAME

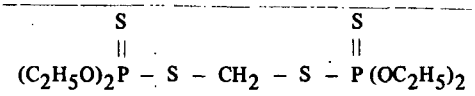
CAS Number: 563-12-2

Chemical Name: Phosphorodithioic acid, 5,5'-methylene O,O,O',O'-tetraethyl ester

Synonyms: 0,0,0',0'-Tetraethyl-S-S-methylene diphosphorodithioate
Tetraethyl-S-S'-methylenedi(phosphorothiolothionate)
Ethyl methylene phosphorodithioate

Molecular Formula: $C_9H_{22}O_4P_2S_4$

Structure:



Chemical Properties

Molecular Weight: 384.5

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point: -13°C

Density: 1.220 at 20°C/4°C

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Gradually oxidizes in air

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 2.0×10^6 lbs.

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	13 mg/kg	rat	oral
	62 mg/kg	rat	skin
	26 mg/kg	rat	intraperitoneal
	55 mg/kg	rat	unreported
	35 mg/kg	mouse	intraperitoneal
	890 mg/kg	rabbit	skin
	45 mg/kg	wild bird	oral

Non-lethal Acute Effects:

Central nervous system			
TD_{Lo}	16 mg/kg	infant	oral
Blood effects			
TD_{Lo}	100 μg/kg	human	oral

Chronic Toxicity

U.S. Occupational Standard:
EPA: Farm worker field re-entry

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethyl acetate

CHEMICAL NAME

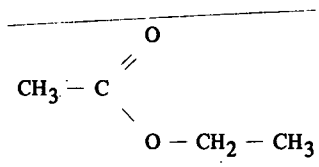
CAS Number: 141-78-6

Chemical Name: Acetic acid, ethyl ester

Synonyms: Acetic ester
Ethylacetic ester
Ethyl etharate
Ethyl esters of acetic acid

Molecular Formula: $C_4H_8O_2$

Structure:



Chemical Properties

Molecular Weight: 88.10

Physical State: Liquid

Vapor Pressure: 92.5 mm at 25°C

Vapor Density: 3.04

Boiling Point: 77.06°C at 760 mm

Melting Point: -83.578°C

Density: 0.8946 at 25°C/4°C

Solubility: Soluble (89 gm/l H_2O)

Octanol/Water Partition Coefficient: 2.68

Environmental Persistence

BOD: 69% of theoretical after 20 days at 20°C
Total theoretical oxygen demand = 1.82 gm/gm

Atmospheric Reactivity:

Safety Hazard:

Ethyl acetate

PRODUCTION DATA

Annual U.S. Production: 212.0 x 10^6 lbs.

Consumption: 212.0 x 10^6 lbs.

Fraction of Dispersion: 0.91

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 196.1

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	5000 mg/kg	rat	subcutaneous
	709 mg/kg	mouse	intraperitoneal
	3000 mg/kg	cat	subcutaneous
	4930 mg/kg	rabbit	oral
	3000 mg/kg	guinea pig	subcutaneous
LC_{50}	1600 mg/kg	rat	inhalation
LC_{Lo}	31 mg/m^3 (1 hour)	mouse	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA : 400 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 400 ppm

Other Chronic Effects:

Irritating to mucous surfaces and eyes
Dermatitis
Congestion of liver and kidneys
Anemia, leucocytosis

Ethyl acetoacetate

CHEMICAL NAME

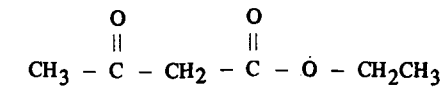
CAS Number: 141-97-9

Chemical Name: Acetoacetic acid, ethyl ester

Synonyms: 3-Oxo-butanoic acid, ethyl ester
Diacetic ether

Molecular Formula: $C_6H_{10}O_3$

Structure:



Chemical Properties

Molecular Weight: 130.15

Physical State: Liquid

Vapor Pressure: 1 mm at 28.5°C

Vapor Density: 4.48

Boiling Point: 180.8°C

Melting Point: <-80°C

Density: 1.0282 at 20°C/4°C

Solubility: Very soluble (H_2O)

Octanol/Water Partition Coefficient: 1.23

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Ethyl acetoacetate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3980 mg/kg	rat	oral

Non-lethal Acute Effects:
Local irritant to skin and mucous membranes

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethyl acrylate

CHEMICAL NAME

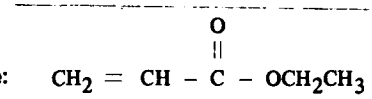
CAS Number: 140-88-5

Chemical Name: Acrylic acid, ethyl ester

Synonyms: Ethyl acrylate
Ethyl propenoate
Propenoic acid, ethyl ester

Molecular Formula: $C_5H_8O_2$

Structure:



Chemical Properties

Molecular Weight: 100.13

Physical State: Liquid

Vapor Pressure: 38.5 mm at 25°C

Vapor Density: 3.45

Boiling Point: 99.8°C

Melting Point: -71.2°C

Density: 0.9234 at 20°C/4°C

Solubility: Slightly soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous
Explosion–dangerous

Ethyl acrylate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	830 mg/kg	rat	oral
	1950 mg/kg	rabbit	skin
LD_{Lo}	420 mg/kg	rabbit	oral
LC_{Lo}	2000 ppm (4 hours)	rat	inhalation
	1204 ppm (7 hours)	rabbit	inhalation
	1204 ppm (7 hours)	guinea pig	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA: 25 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 25 ppm

Other Chronic Effects:

Irritation of gastrointestinal tract
Degenerative changes in cardiac, hepatic, renal, and splenic tissues
Skin and eye irritant

Ethyl alcohol

CHEMICAL NAME

CAS Number: 64-17-5

Chemical Name: Ethanol

Synonyms:
Absolute ethanol
Anhydrous alcohol
Dehydrated alcohol
Ethyl hydrate
Ethyl hydroxide
Methyl carbinol
Alcohol

Molecular Formula: C_2H_6O

Structure: CH_3CH_2OH

Chemical Properties

Molecular Weight: 46.07

Physical State: Liquid

Vapor Pressure: 54.3 mm at 25°C

Vapor Density: 1.59

Boiling Point: 78.5°C

Melting Point: -117.3°C

Density: 0.7893 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient: 0.38

Environmental Persistence

BOD: 84% at 20°C for 20 days
Total theoretical 2.10 gm/gm

Atmospheric Reactivity:
Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous
Explosion–moderate

Ethyl alcohol

PRODUCTION DATA

Annual U.S. Production: 1850.6 x 10^6 lbs.

Consumption: 1582.6 x 10^6 lbs.

Fraction of Dispersion: 0.35

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 581.7

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1440 mg/kg	rat	intravenous
	8285 mg/kg	mouse	subcutaneous
	1973 mg/kg	mouse	intravenous
	6300 mg/kg	rabbit	oral
	5560 mg/kg	guinea pig	oral
LD_{Lo}	2000 mg/kg	child	oral
	6000 mg/kg	human	oral
	1225 mg/kg	rat	intraperitoneal
	220 mg/kg	mouse	oral
LD_{100}	5500 mg/kg	dog	oral
	3000 mg/kg	dog	oral
	5000 mg/kg	dog	subcutaneous
	1600 mg/kg	dog	intravenous
	6000 mg/kg	cat	oral
	5000 mg/kg	rabbit	intravenous
	3500 mg/kg	rabbit	intraperitoneal
Non-lethal Acute Effects:			
Gastrointestinal			
TD_{Lo}	50 mg/kg	human	oral
CNS			
TD_{Lo}	1400 mg/kg	human	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Irritation of eyes and mucous membranes
CNS depressant

Ethylamine

CHEMICAL NAME

CAS Number: 75-04-7

Chemical Name: Ethanamine

Synonyms: Aminoethane
Monoethylamine

Molecular Formula: C_2H_7N

Structure: $CH_3 - CH_2 - NH_2$

Chemical Properties

Molecular Weight: 45.08

Physical State: Liquid

Vapor Pressure: 1094.24 mm at 25°C

Vapor Density:

Boiling Point: 16.6° at 760 mm

Melting Point: -81°C

Density: 0.6829 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient: -0.27

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous

PRODUCTION DATA

Annual U.S. Production: 45.9×10^6 lbs.

Consumption: 45.9×10^6 lbs.

Fraction of Dispersion: 0.30

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 14.4

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	390 mg/kg	rabbit	skin
LD_{Lo}	400 mg/kg	rat	oral
LC_{Lo}	3000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Irritation of eyes, skin, and respiratory tract

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 10 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethyl sec-amyl ketone

CHEMICAL NAME

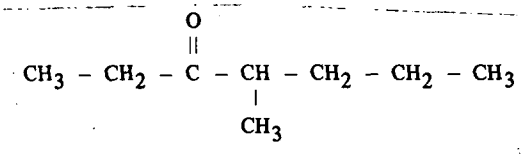
CAS Number: 6137-11-7

Chemical Name: 4-Methyl-3-heptanone

Synonyms: Ethyl sec-amyl ketone

Molecular Formula: $C_8H_{16}O$

Structure:



Chemical Properties

Molecular Weight: 128.22

Physical State:

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point:

Density:

Solubility:

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Ethyl sec-amyl ketone

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3500 mg/kg	rat	oral
	3800 mg/kg	mouse	oral
	2500 mg/kg	guinea pig	oral
LC_{Lo}	3484 ppm (8 hours)	rat	inhalation
	3484 ppm (8 hours)	mouse	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA: 25 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethylbenzene

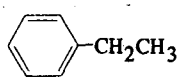
CHEMICAL NAME

CAS Number: 100-41-4

Chemical Name: Ethylbenzene

Synonyms: Ethylbenzol
Phenylethane

Molecular Formula: C_8H_{10}

Structure: 

Chemical Properties

Molecular Weight: 106.17

Physical State: Liquid

Vapor Pressure: 9.63 mm at 25°C

Vapor Density: 3.66

Boiling Point: 136.2°C at 760 mm

Melting Point: -94.97°C

Density: 0.8670 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient: 3.15

Environmental Persistence

BOD: 3% of theoretical after 5 days at 20°C
Total theoretical oxygen demand 3.16 gm/gm

Atmospheric Reactivity:
Occurs in atmosphere in small quantities
Unreactive to RO_2 and O_3
Reacts with oxidizing materials
Activity toward OH: $t_{1/2}$ = 0.8 days, product is hydroxyethylbenzene

Safety Hazard:
Fire–moderate

Ethylbenzene

PRODUCTION DATA

Annual U.S. Production: 6920 x 10^6 lbs. (1975:4,008.2 x 10^6 lbs.)

Consumption: 6713 x 10^6 lbs.

Fraction of Dispersion: 0.02

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 203.5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3500 mg/kg	rat	oral
LC_{Lo}	4000 ppm (4 hours)	rat	inhalation
	1000 ppm	guinea pig	inhalation
Non-lethal Acute Effects:			
Irritant			
TC_{Lo}	1000 ppm	human	subcutaneous
Narcosis			
Dermatitis			

Chronic Toxicity

U.S. Occupational Standard: TWA: 100 ppm

Carcinogenicity: Negative for inhalation and ingestion

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:
- Blood disorders after repeated doses
- Conjunctivitis and corneal erosion
- Vertigo–2000 ppm (5 minutes)

Ethyl bromide

CHEMICAL NAME

CAS Number: 74-96-4

Chemical Name: Bromoethane

Synonyms: Bromic ether
Hydrobromic ether

Molecular Formula: C_2H_5Br

Structure: CH_3CH_2Br

Chemical Properties

Molecular Weight: 108.98

Physical State: Volatile liquid

Vapor Pressure: 482.76 mm at 25°C

Vapor Density: 3.76

Boiling Point: 38.4°C

Melting Point: -118.6°C

Density: 1.451 at 20°C/4°C

Solubility: Slightly soluble (H_2O)

Octanol/Water Partition Coefficient: 1.74

Environmental Persistence

BOD:

Atmospheric Reactivity:
Reacts with oxidizing materials to produce hydrobromic acid and bromide

Safety Hazard:
Explosion–moderate
Disaster hazard–dangerous, toxic fumes of bromine

Ethyl bromide

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LC_{Lo}	2200 ppm	guinea pig	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA: 200 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 200 ppm

Other Chronic Effects:

Irritant to mucous membranes, especially lungs, liver, and kidney damage

Ethyl butyl ketone

CHEMICAL NAME

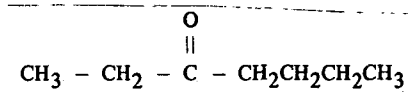
CAS Number: 106-35-4

Chemical Name: 3-Heptanone

Synonyms: Ethyl butyl ketone

Molecular Formula: $C_7H_{14}O$

Structure:



Chemical Properties

Molecular Weight: 114.19

Physical State: Liquid

Vapor Pressure: <1 mm at 20°C

Vapor Density: 3.93

Boiling Point: 148°C

Melting Point: -39°C

Density: 0.8183 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–moderate

Ethyl butyl ketone

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2760 mg/kg	rat	oral
LC_{Lo}	2000 ppm (4 hours)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA: 50 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 50 ppm

Other Chronic Effects:

Ethyl cellulose

CHEMICAL NAME

CAS Number: 9004-57-3

Chemical Name: Cellulose, ethyl ether

Synonyms: Ethyl ether of cellulose
Cellulose ethylate
Cellulose ethyl

Molecular Formula: (Exact composition unknown or undetermined)

Structure: (Exact composition unknown or undetermined)

Chemical Properties

Molecular Weight:	Physical State: Solid
Vapor Pressure:	Vapor Density:
Boiling Point:	Melting Point: 240 to 255°C
Density: 1.07 to 1.18	Solubility: Insoluble (H_2O)
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Ethyl cellulose

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethyl chloride

CHEMICAL NAME

CAS Number: 75-00-3

Chemical Name: Chloroethane

Synonyms: Muriatic acid
Hydrochloric ether

Molecular Formula: C_2H_5Cl

Structure: $CH_3CH_2 - Cl$

Chemical Properties

Molecular Weight: 64.52

Physical State: Liquid or gas

Vapor Pressure: 20 mm at 21°C

Vapor Density: 2.22

Boiling Point: 12.27°C at 760 mm

Melting Point: -136.4°C

Density: 0.8978 at 20°C/4°C

Solubility: Slightly soluble (0.574 gm/100 ml H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Reacts with oxidizing materials
RO_2: $t_{1/2}$ = 2000 years
OH: $t_{1/2}$ = 10 years
O_3: $t_{1/2}$ = 1 year

Safety Hazard:
Fire–very dangerous
Explosion–very dangerous
Disaster hazard –very dangerous, toxic fumes of phosgene

Ethyl chloride

PRODUCTION DATA

Annual U.S. Production: 660 x 10^6 lbs. (1974)

Consumption: 660 x 10^6 lbs.

Fraction of Dispersion: 0.05

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 34.5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
Non-lethal Acute Effects:			
CNS			
TC_{Lo}	13,000 ppm	human	inhalation
Irritant to eyes			
Kidney, heart, and liver damage			
Subcutaneous tissue edema			
Leucocytosis			

Chronic Toxicity

U.S. Occupational Standard: (air) TWA: 1000 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 1000 ppm

Other Chronic Effects:

Ethyl chloroacetate

CHEMICAL NAME

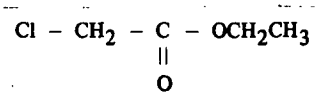
CAS Number: 105-39-5

Chemical Name: Chloroacetic acid, ethyl ester

Synonyms: Ethylchloroethanoate
Chloro-α-acetic acid, ethyl ester
Ethyl chloroacetate

Molecular Formula: $C_4H_7ClO_2$

Structure:



Chemical Properties

Molecular Weight: 122.55

Physical State: Liquid

Vapor Pressure: 4.93 mm at 25°C

Vapor Density: 4.3

Boiling Point: 143.6°C

Melting Point: -26°C

Density: 1.1585 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate
Disaster hazard–dangerous, toxic fumes–chlorides

Ethyl chloroacetate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Non-lethal Acute Effects:
Local irritant to eyes

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethyl cyanoacetate

CHEMICAL NAME

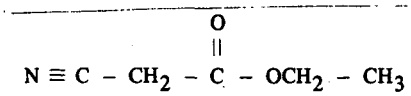
CAS Number: 105-56-6

Chemical Name: Cyanoacetic acid, ethyl ester

Synonyms: Malonic ethyl ester nitrile

Molecular Formula: $C_5H_7NO_2$

Structure:



Chemical Properties

Molecular Weight: 113.1

Physical State: Liquid

Vapor Pressure: 67.8°C

Vapor Density: 3.9

Boiling Point: 206°C

Melting Point: -22.5°C

Density: 1.0654 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:

Fire–slight

Disaster hazard–dangerous, toxic fumes of cyanides

Ethyl cyanoacetate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	750 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethylene

CHEMICAL NAME

CAS Number: 74-85-1

Chemical Name: Ethylene

Synonyms: Acetene
Ethene

Molecular Formula: C_2H_4

Structure: $H_2C = CH_2$

Chemical Properties

Molecular Weight: 28.06

Physical State: Gas

Vapor Pressure: 34,200 mm at 0°C

Vapor Density: 0.98

Boiling Point: -103.9°C at 760 mm

Melting Point: -169°C

Density: 0.99267 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Reported in air in concentrations of 0.012 to 0.25 ppm
Activity: unresistive to RO_2; $t_{1/2}$ with O_3 = <4 hours
Activity toward OH: $t_{1/2}$ = 1 day

Safety Hazard: Fire–dangerous
Explosion–moderate

PRODUCTION DATA

Annual U.S. Production: 20,852.1 x 10^6 lbs.

Consumption: 20,852.1 x 10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 521.3

TOXICITY DATA

Acute Toxicity **Dosage** **Animal** **Route**

Paralysis at high concentrations
Malfunctions of heart
Depressed activity of sympathetic ganglion of upper neck (cat)
Increased blood coagulation time (mouse)
Disturbances of the electrical activity of the brain (dog)

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: **TLV:**

Other Chronic Effects: Lung inflamation; histopathological changes in liver and cerebellum (rabbit); peripheral leucopenia; reduced cellularity of the bone marrow, hypertension, inhibition of chlolinesterase activity, disruption of subordination chronaxy (rat).

Ethylene carbonate

CHEMICAL NAME

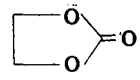
CAS Number: 96-49-1

Chemical Name: 1,3-Dioxolan-2-one

Synonyms: Glycol carbonate
Dioxolone-2

Molecular Formula: $C_3H_4O_3$

Structure:



Chemical Properties

Molecular Weight: 88.06

Physical State: Solid

Vapor Pressure: 0.01 mm at 20°C

Vapor Density: 3.04

Boiling Point: 248°C at 760 mm

Melting Point: 39 to 40°C

Density: 1.322 at 39°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–slight

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethylene chlorohydrin

CHEMICAL NAME

CAS Number: 107-07-3

Chemical Name: 2-Chloroethanol

Synonyms: Ethylene chlorohydrin
β-Chloroethyl alcohol
Glycol chlorohydrin

Molecular Formula: C_2H_5ClO

Structure: $Cl - CH_2 - CH_2OH$

Chemical Properties

Molecular Weight: 80.52

Physical State: Liquid

Vapor Pressure: 7.65 mm at 25°C

Vapor Density: 2.78

Boiling Point: 128.8°C at 760 mm

Melting Point: -67.5°C

Density: 1.2003 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate
Disaster hazard–dangerous–toxic fumes–phosgene

Ethylene chlorohydrin

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	580 mg/kg	rat	oral
	84 mg/kg	rat	subcutaneous
	81 mg/kg	mouse	oral
	81 mg/kg	mouse	intraperitoneal
	56 mg/kg	rabbit	skin
	67 mg/kg	rabbit	intraperitoneal
	110 mg/kg	guinea pig	oral
	71 mg/kg	guinea pig	intraperitoneal
Ingestion has caused human death			
LD_{Lo}	40 mg/kg	rat	intraperitoneal
	1450 mg/kg	mouse	skin
	100 mg/kg	rabbit	intravenous
	70 mg/kg	guinea pig	skin
	250 mg/kg	frog	subcutaneous
LC_{50}	385 mg/m^3	mouse	inhalation
LC_{Lo}	32 ppm (4 hours)	rat	inhalation
	3000 mg/m^3 (112 minutes)	guinea pig	inhalation
Non-lethal Acute Effects:			
Skin–TD_{Lo}	5000 mg/kg	human	skin
Nausa			
Irritation of eyes			
Convulsions			

Chronic Toxicity

U.S. Occupational Standard: (air) 5 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 5 ppm (skin)

Other Chronic Effects:

Ethylenediamine

CHEMICAL NAME

CAS Number: 107-15-3

Chemical Name: Ethylenediamine

Synonyms: 1,2-Ethanediamine
1,2-Diaminoethane

Molecular Formula: $C_2H_8N_2$

Structure: $H_2N - CH_2 - CH_2 - NH_2$

Chemical Properties

Molecular Weight: 60.10

Physical State: Liquid

Vapor Pressure: 13.04 mm at 25°C

Vapor Density: 2.07

Boiling Point: 116.5°C at 760 mm

Melting Point: 8.5°C

Density: 0.8994 at 20°C/4°C

Solubility: Very soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 70% of theoretical after 20 days at 20°C
Total theoretical oxygen demand = 3.7 gm/gm

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Ethylenediamine

PRODUCTION DATA

Annual U.S. Production: 54.4 x 10^6 lbs.

Consumption: 43.3 x 10^6 lbs.

Fraction of Dispersion: 0.50

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 22.5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	760 mg/kg	rat	oral
	424 mg/kg	mouse	subcutaneous
	730 mg/kg	rabbit	skin
	470 mg/kg	guinea pig	oral
	4000 ppm (8 hours)	rat	inhalation

Non-lethal Acute Effects:

Irritant			
TC_{Lo}	200 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 10 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 10 ppm

Other Chronic Effects: Allergen
Dermatitis
Asthmatic

Ethylene dibromide

CHEMICAL NAME

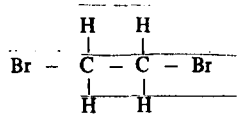
CAS Number: 106-93-4

Chemical Name: 1,2-Dibromoethane

Synonyms: Ethylene dibromide
Glycol dibromide
EDB

Molecular Formula: $C_2H_4Br_2$

Structure:



Chemical Properties

Molecular Weight: 187.88

Physical State: Heavy liquid

Vapor Pressure: 14.54 mm at 25°C

Vapor Density: 6.48

Boiling Point: 131.36°C at 760 mm

Melting Point: 9.79°C

Density: 2.1707 at 25°C/4°C

Solubility: Slightly (H_2O)
(0.431 gm/100 ml at 30°C)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Photochemical degradation: decomposes

Safety Hazard:

Ethylene dibromide

PRODUCTION DATA

Annual U.S. Production: 315.5 x 10^6 lbs.

Consumption: 315.5 x 10^6 lbs.

Fraction of Dispersion: 0.95

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 304.4

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	140 mg/kg	rat	oral
	146 mg/kg	mouse	unreported
	55 mg/kg	rabbit	oral
	300 mg/kg	rabbit	skin
	110 mg/kg	guinea pig	oral
	79 mg/kg	chicken	oral
LD_{Lo}	250 mg/kg	mouse	oral
LC_{Lo}	400 ppm (2 hours)	rat	inhalation
	6425 ppm (1 hour)	rabbit	inhalation
	400 ppm (3 hours)	guinea pig	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air): TWA 20 ppm
ceiling 30 ppm
peak 50 ppm/5 mins/8 hours

Carcinogenicity: Positive, 10 week incubation, mouse

Mutagenicity: Positive in bacteria

Teratogenicity:

TLV:

Other Chronic Effects: Abnormal sperm
Reduced sperm count
Skin irritation and blisters
Lung stimulation

Ethylene dichloride

CHEMICAL NAME

CAS Number: 107-06-2

Chemical Name: 1,2-Dichloroethane

Synonyms: Ethylene dichloride
Ethylene chloride

Molecular Formula: $C_2H_4Cl_2$

Structure: $Cl - CH_2 - CH_2 - Cl$

Chemical Properties

Molecular Weight: 99.0

Vapor Pressure: 84.42 mm at 25°C

Boiling Point: 83.5°C at 760 mm

Density: 1.257 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 3.35

Melting Point: -35.5°C

Solubility: Slightly soluble (H_2O)
(0.43 gm/100 ml)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–dangerous
Explosion–moderate

Ethylene dichloride

PRODUCTION DATA

Annual U.S. Production: 9,293 x 10^6 lbs. (1973)

Consumption: ca. 8,921.3 x 10^6 lbs.

Fraction of Dispersion: 0.05

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 540.2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	860 mg/kg	rabbit	oral
	680 mg/kg	rat	oral
LD_{Lo}	845 mg/kg	human	oral
	600 mg/kg	rat	intraperitoneal
	500 mg/kg	rat	subcutaneous
	600 mg/kg	mouse	oral
	250 mg/kg	mouse	intraperitoneal
	380 mg/kg	mouse	subcutaneous
	2000 mg/kg	dog	oral
	175 mg/kg	dog	intravenous
	1200 mg/kg	rabbit	subcutaneous
LC_{Lo}	1000 ppm (4 hours)	rat	inhalation
	5000 mg/m^3 (2 hours)	mouse	inhalation
	3000 ppm (7 hours)	rabbit	inhalation
	3000 ppm (7 hours)	pig	inhalation
	1500 ppm (7 hours)	guinea pig	inhalation
Non-lethal Acute Effects:			
Central nervous system			
TC_{Lo}	4000 ppm (hour)	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 50 ppm
Ceiling 100 ppm
Peak 200 ppm/5 minute/3 hours

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethylene glycol

CHEMICAL NAME

CAS Number: 107-21-1

Chemical Name: Ethylene glycol

Synonyms: 1,2-Ethyanediol
Ethylene alcohol

Molecular Formula: $C_2H_6O_2$

Structure: HO – CH_2 – CH_2 – OH

Chemical Properties

Molecular Weight: 62.1

Physical State: Liquid

Vapor Pressure: 0.05 mm at 20°C

Vapor Density: 2.14

Boiling Point: 198°C at 760 mm

Melting Point: -11.5°C

Density: 1.1088 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient: -1.88

Environmental Persistence

BOD: 13% Theoretical

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–slight
Explosion–moderate

Ethylene glycol

PRODUCTION DATA

Annual U.S. Production: 3,761.1 x 10^6 lbs.

Consumption: 3,242 x 10^6 lbs. (1974)

Fraction of Dispersion: 0.70

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2,526.3

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2000 mg/kg	cat	oral
	6610 mg/kg	guinea pig	oral
LD_{Lo}	1500 mg/kg	human	oral
	2700 mg/kg	mouse	skin
	1000 mg/kg	rabbit	intraperitoneal

Non-lethal Acute Effects:

CNS stimulation followed by depression, if ingested
Kidney damage
Very toxic in particulate form

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplastic effects: TD_{Lo} 4 gm/kg mouse skin

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects: Slight irritant

Ethylene glycol, diacetate

CHEMICAL NAME

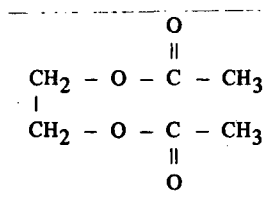
CAS Number: 111-55-7

Chemical Name: Ethylene glycol, diacetate

Synonyms: Ethylene diacetate
Gylcol diacetate

Molecular Formula: $C_6H_{10}O_4$

Structure:



Chemical Properties

Molecular Weight: 146.14

Physical State: Liquid

Vapor Pressure: 1 mm at 38.3°C

Vapor Density: 5.04

Boiling Point: 190°C at 760 mm

Melting Point: -31.0°C

Density: 1.1063 at 20°C/20°C

Solubility: Very soluble (H_2O)

Octanol/Water Partition Coefficient: 0.38

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing material

Safety Hazard: Fire–moderate

Ethylene glycol, diacetate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1070 mg/kg	mouse	intarperitoneal
	4940 mg/kg	guinea pig	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethylene glycol, dibutyl ether

CHEMICAL NAME

CAS Number: 112-48-1

Chemical Name: 1,2-Dibutoxyethane

Synonyms: Dibutyl cellosolve

Molecular Formula: $C_{10}H_{22}O_2$

Structure: $CH_3 - (CH_2)_3 - O - CH_2 - CH_2 - O - (CH_2)_3 - CH_3$

Chemical Properties

Molecular Weight: 174.29

Physical State: Liquid

Vapor Pressure: 0.09 mm at 20°C

Vapor Density:

Boiling Point: 203.1°C at 760 mm

Melting Point: -69.1°C

Density: 0.8374 at 20°C/20°C

Solubility: Slightly soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Ethylene glycol, dibutyl ether

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethylene glycol, diethyl ether

CHEMICAL NAME

CAS Number: 16484-86-9

Chemical Name: Ethylene glycol, diethyl ether

Synonyms: 1,2-Diethoxyethane
Diethyl cellosolve

Molecular Formula: $C_6H_{14}O_2$

Structure: $CH_3CH_2OCH_2CH_2OCH_2CH_3$

Chemical Properties

Molecular Weight: 118.18

Physical State: Liquid

Vapor Pressure: 9.4 mm at 20°C

Vapor Density:

Boiling Point: 123.5°C at 760 mm

Melting Point: -74°C

Density: 0.8484 at 20°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Ethylene glycol, diethyl ether

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	4390 mg/kg	rat	oral
	2440 mg/kg	guinea pig	oral
LC_{Lo}	9000 ppm (14 hours)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethylene glycol, dimethyl ether

CHEMICAL NAME

CAS Number: 534-15-6

Chemical Name: Dimethyl acetal acetaldehyde

Synonyms: Ethylene glycol, dimethyl ether
GDME
1,2-Dimethoxyethane

Molecular Formula: $C_4H_{10}O_2$

Structure: $CH_3 - O - CH_2CH_2 - O - CH_3$

Chemical Properties

Molecular Weight: 90.14

Physical State: Liquid

Vapor Pressure: 77.52 mm at 25°C

Vapor Density: 3.11

Boiling Point: 83 to 84°C at 760 mm

Melting Point: -58°C

Density: 0.8629 at 20°C/4°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous
Explosion–dangerous

Ethylene glycol, dimethyl ether

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethylene glycol, monoacetate

CHEMICAL NAME

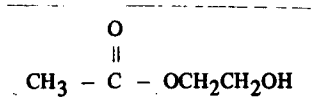
CAS Number: 542-59-6

Chemical Name: Ethylene glycol, monoacetate

Synonyms: Glycol monoacetate
1,2-Ethanediol, monoacetate
Hydroxyethyl acetate

Molecular Formula: $C_4H_8O_3$

Structure:



Chemical Properties

Molecular Weight: 104.10

Physical State: Liquid

Vapor Pressure:

Vapor Density: 3.59

Boiling Point: 181 to 182°C

Melting Point:

Density: 1.108 at 15°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Ethylene glycol, monoacetate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1310 mg/kg	mouse	intraperitoneal
	3800 mg/kg	guinea pig	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethylene glycol, monobutyl ether

CHEMICAL NAME

CAS Number: 111-76-2

Chemical Name: 2-Butoxyethanol

Synonyms: Ethylene glycol, monobutyl ether
Butyl cellosolve

Molecular Formula: $C_6H_{14}O_2$

Structure: $CH_3(CH_2)_3 - O - CH_2CH_2OH$

Chemical Properties

Molecular Weight: 118.17

Physical State: Liquid

Vapor Pressure: 0.76 mm at 20°C

Vapor Density: 4.07

Boiling Point: 171.2°C

Melting Point:

Density: 0.9027 at 20°C/4°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–moderate

Ethylene glycol, monobutyl ether

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1480 mg/kg	rat	oral
	550 mg/kg	rat	intraperitoneal
	340 mg/kg	rat	intravenous
	1230 mg/kg	mouse	oral
	536 mg/kg	mouse	intraperitoneal
	1130 mg/kg	mouse	intravenous
	320 mg/kg	rabbit	oral
	560 mg/kg	rabbit	skin
	280 mg/kg	rabbit	intravenous
	1200 mg/kg	guinea pig	oral
	230 mg/kg	guinea pig	skin
LC_{50}	700 ppm (2 hours)	mouse	inhalation
	500 ppm (4 hours)	rat	inhalation
Non-lethal Acute Effects:			
Irritant			
TD_{Lo}	195 ppm (8 hours)	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 50 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 50 ppm (skin)

Other Chronic Effects:

Ethylene glycol, monoethyl ether

CHEMICAL NAME

CAS Number: 110-80-5

Chemical Name: 2-Ethoxyethanol

Synonyms: Cellosolve solvent
Ethylene glycol, monoethyl ether

Molecular Formula: $C_4H_{10}O_2$

Structure: $CH_3CH_2OCH_2CH_2OH$

Chemical Properties

Molecular Weight: 90.12

Physical State: Liquid

Vapor Pressure: 3.8 mm at 20°C

Vapor Density: 3.10

Boiling Point: 135.1°C

Melting Point: <37.7°C (pour point)

Density: 0.9360 at 15°C/15°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate
Explosion–moderate

Ethylene glycol, monoethyl ether

PRODUCTION DATA

Annual U.S. Production: 205.4 x 10^6 lbs

Consumption: 200.4 x 10^6 lbs.

Fraction of Dispersion: 0.97

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 197.5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3000 mg/kg	rat	oral
	4300 mg/kg	mouse	oral
	1710 mg/kg	mouse	intraperitoneal
	3100 mg/kg	rabbit	oral
	1400 mg/kg	guinea pig	oral
LC_{Lo}	4000 ppm (4 hours)	rat	inhalation
	1820 ppm	mouse	inhalation

Non-lethal Acute Effects:

Local irritant
Exposure to vapor produces congestion and edema of the lungs and congestion of the kidney
Eye irritation observed in humans

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 200 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 200 ppm (skin)

Other Chronic Effects:

Ethylene glycol, monoethyl ether acetate

CHEMICAL NAME

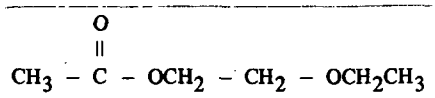
CAS Number: 111-15-9

Chemical Name: 2-Ethoxyethanol acetate

Synonyms: Ethylene glycol, monoethyl ether acetate

Molecular Formula: $C_6H_{12}O_3$

Structure:



Chemical Properties

Molecular Weight: 132.17	**Physical State:** Liquid
Vapor Pressure: 1.2 mm at 20°C	**Vapor Density:** 4.72
Boiling Point: 156.3°C	**Melting Point:** -61.7°C
Density: 0.9748 at 20°C/20°C	**Solubility:** Soluble (H_2O)
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–moderate
Explosion–moderate

Ethylene glycol, monoethyl ether acetate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1420 mg/kg	mouse	intraperitoneal
	1910 mg/kg	guinea pig	oral
LC_{Lo}	1500 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:
Irritation of eyes and respiratory tract

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppm (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Ethylene glycol, monohexyl ether

CHEMICAL NAME

CAS Number: 112-25-4

Chemical Name: 2-(Hexyloxy) ethanol

Synonyms: Ethylene glycol, monohexyl ether
Hexyl cellosolve

Molecular Formula: $C_8H_{18}O_2$

Structure: $HO - CH_2 - CH_2-O - (CH_2)_5CH_3$

Chemical Properties

Molecular Weight: 146.22

Physical State: Liquid

Vapor Pressure: 0.05 mm at 20°C

Vapor Density: 5.04

Boiling Point:

Melting Point: -50.1°C

Density: 0.8894 at 20°C/20°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Ethylene glycol, monohexyl ether

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1480 mg/kg	rat	oral
	896 mg/kg	rabbit	skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethylene glycol, monomethyl ether

CHEMICAL NAME

CAS Number: 109-86-4

Chemical Name: 2-Methoxyethanol

Synonyms: Ethylene glycol, monomethyl ether
Cellosolve acetate
Methyl cellosolve
Ethoxyacetate

Molecular Formula: $C_3H_8O_2$

Structure: $CH_3OCH_2CH_2OH$

Chemical Properties

Molecular Weight: 76.09

Physical State: Liquid

Vapor Pressure: 6.2 at 20°C

Vapor Density: 2.62

Boiling Point: 124.5°C

Melting Point: -81.5°C

Density: 0.9660 at 20°C/4°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Ethylene glycol, monomethyl ether

PRODUCTION DATA

Annual U.S. Production: 137.4 x 10^6 lbs. (1968)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2460 mg/kg	rat	oral
	2140 mg/kg	rat	intravenous
	890 mg/kg	rabbit	oral
	1340 mg/kg	rabbit	skin
	950 mg/kg	guinea pig	oral
LC_{50}	1340 mg/kg	rabbit	inhalation
LC_{Lo}	2000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Central nervous system

TC_{Lo}	25 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 25 ppm (skin)

Other Chronic Effects:

Disturbances of hemopoietic system with or without neurological signs or symptoms
Severe aplastic anemia with tremors and marked mental dullness
Reduction of number of blood platelets and macrocytic anemia

Ethylene glycol, monomethyl ether acetate

CHEMICAL NAME

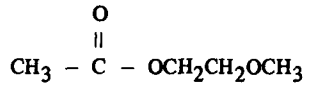
CAS Number: 110-49-6

Chemical Name: 2-Methoxyethanol acetate

Synonyms: Ethylene glycol, monomethyl ether acetate
Cellosolve acetate

Molecular Formula: $C_5H_{10}O_3$

Structure:



Chemical Properties

Molecular Weight: 118.13

Physical State: Liquid

Vapor Pressure: 1.2 mm at 20°C

Vapor Density: 4.07

Boiling Point: 145°C

Melting Point: -65.1°C

Density: 1.0067 at 20°C/20°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Ethylene glycol, monomethyl ether acetate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3390 mg/kg	rat	oral
	1250 mg/kg	guinea pig	oral
LC_{Lo}	7000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Irritation of eyes and respiratory tract
Nausea and vomiting

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 25 ppm (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 25 ppm

Other Chronic Effects:

Ethylene glycol, monooctyl ether

CHEMICAL NAME

CAS Number: 10020-43-6

Chemical Name: 2-(Octyloxy)ethanol

Synonyms: Ethylene glycol monooctyl ether

Molecular Formula: $C_{10}H_{22}O_2$

Structure: $CH_3(CH_2)_7 - O - CH_2 - CH_2 - OH$

Chemical Properties

Molecular Weight: 174.28	**Physical State:** Liquid
Vapor Pressure: 0.02 mm at 20 C	**Vapor Density:**
Boiling Point: 228.3°C	**Melting Point:**
Density: 0.8859 at 20°C	**Solubility:**
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–slight
Explosion–moderate

Ethylene glycol, monooctyl ether

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethylene glycol, monophenyl ether

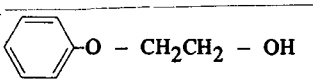
CHEMICAL NAME

CAS Number: 122-99-6

Chemical Name: 2-Phenoxyethanol

Synonyms: Ethylene glycol, monophenyl ether
Phenyl cellosolve

Molecular Formula: $C_8H_{10}O_2$

Structure: 

Chemical Properties

Molecular Weight: 138.2

Physical State: Liquid

Vapor Pressure: <0.01 mm at 20°C

Vapor Density: 4.76

Boiling Point: 244.9°C

Melting Point: 14°C

Density: 1.1094 at 20°C/20°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient: 1.16

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–slight
Explosion–moderate

Ethylene glycol, monophenyl ether

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1260 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethylene glycol, monopropyl ether

CHEMICAL NAME

CAS Number: 2807-30-9

Chemical Name: 2-Propoxyethanol

Synonyms: Propyl cellosolve
Ethylene glycol monopropyl ether

Molecular Formula: $C_5H_{12}O_2$

Structure: $HO - CH_2 - CH_2 - O - CH_2 - CH_2 - CH_3$

Chemical Properties

Molecular Weight: 104.14

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 150°C at 743 mm

Melting Point:

Density: 0.9112 at 20°C/4°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–moderate

Ethylene glycol, monopropyl ether

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	4890 mg/kg	rat	oral
	940 mg/kg	rabbit	skin
LC_{Lo}	2000 ppm (4 hours)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethyleneimine

CHEMICAL NAME

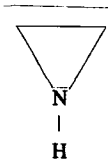
CAS Number: 151-56-4

Chemical Name: Ethylenimine

Synonyms: Aziridine

Molecular Formula: C_2H_5N

Structure:



Chemical Properties

Molecular Weight: 43.07

Physical State: Liquid

Vapor Pressure: 160 mm at 20°C

Vapor Density: 1.48

Boiling Point: 56°C at 756 mm

Melting Point: -78°C

Density: 0.832 at 20°C/4°C

Solubility: Infinitely soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–dangerous
Explosion–dangerous

PRODUCTION DATA

Annual U.S. Production: 5×10^6 lbs.

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 0.08

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	15 mg/kg	rat	oral
	3800 mg/kg	rat	intraperitoneal
	15 mg/kg	mouse	unreported
	14 mg/kg	guinea pig	skin
LC_{Lo}	25 ppm (8 hours)	rat	inhalation
	25 ppm (8 hours)	guinea pig	inhalation
LC_{50}	400 mg/m^3	mouse	inhalation
	2200 ppm (10 mins)	rat	inhalation

Non-lethal Acute Effects:
Skin irritation
Skin sensitization
Necrosis of cornea
Nausea and vomiting

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 1 mg/m^3 (skin)

Carcinogenicity:			
TD_{Lo}	20 mg/kg (67 days)	rat	subcutaneous
	235 mg/kg (76 weeks)	mouse	oral
Mutagenicity:			
TD_{Lo}	6 mg/kg	mouse	intraperitoneal

Teratogenicity:

TLV:
Odor perception: 2 ppm

Other Chronic Effects:

Ethylene oxide

CHEMICAL NAME

CAS Number: 75-21-8

Chemical Name: Ethylene oxide

Synonyms: 1,2-Epoxyethane
Oxirane

Molecular Formula: C_2H_4O

Structure:

Chemical Properties

Molecular Weight: 44.05

Physical State: Gas

Vapor Pressure: 1475 mm at 25°C

Vapor Density: 1.52

Boiling Point: 13.5°C at 746 mm

Melting Point: -111.3°C

Density: 0.8711 at 20°C/20°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 31% of theoretical after 10 days at 70°C at 100 mg/ml
Total theoretical oxygen demand = 1.82 gm/gm

Atmospheric Reactivity:
Unreactive to RO_2 or O_3
Activity towards OH: $t_{1/2}$ = 1.6 days
Reacts with oxidizing materials
Hydrolyzes rapidly: $t_{1/2}$ = 2.5 days at pH 7

Safety Hazard: Fire–dangerous
Explosion–severe

PRODUCTION DATA

Annual U.S. Production: 3,961.8 x 10^6 lbs.

Consumption: 3,934.0 x 10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 98.8

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	330 mg/kg	rat	oral
	270 mg/kg	guinea pig	oral
LC_{50}	1462 ppm (4 hours)	rat	inhalation
	836 ppm (4 hours)	mouse	inhalation
	960 ppm (4 hours)	dog	inhalation
LC_{Lo}	7000 ppm (150 minutes)	guinea pig	inhalation
LC	15,000 to 10,000 ppm (air)	most animals	inhalation

Non-lethal Acute Effects:

Irritant to eyes and mucous membranes
Pulmonary edema at high concentrations
Reduced motor response–CNS damage
Skin burns

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 50 ppm

Carcinogenicity: Positive carcinogen in mice–various tumors–oral

Mutagenicity:

Increased chromosomal aberrations

TD_{Lo}	30 mg/m^3	mammal	inhalation

Teratogenicity: **TLV:** 50 ppm

Other Chronic Effects:

Ethyl ether

CHEMICAL NAME

CAS Number: 60-29-7

Chemical Name: Ethyl ether

Synonyms: Ether
Ethyl oxide
Anaesthesia ether
Diethyl ether
1,1'-Oxybis-ethane

Molecular Formula: $C_4H_{10}O$

Structure: $CH_3 - CH_2 - O - CH_2 - CH_3$

Chemical Properties

Molecular Weight: 74.12

Physical State: Volatile liquid

Vapor Pressure: 442 mm at 20°C

Vapor Density: 2.56

Boiling Point: 34.5°C

Melting Point: -116.2°C

Density: 0.7135 at 20°C/4°C

Solubility: Slightly soluble (H_2O)

Octanol/Water Partition Coefficient: 0.93

Environmental Persistence

BOD: 1% theoretical

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous
Explosion–severe

PRODUCTION DATA

Annual U.S. Production: 103.2 x 10^6 lbs. (1969)

Consumption: 102. x 10^6 lbs.

Fraction of Dispersion: 0.50

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 35.7

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1700 mg/kg	rat	oral
LD_{Lo}	2000 mg/kg	rat	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard: (air) TWA: 400 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 400 ppm

Other Chronic Effects:
CNS depressant

Ethyl formate

CHEMICAL NAME

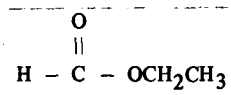
CAS Number: 109-94-4

Chemical Name: Formic acid, ethyl ester

Synonyms: Formic ether
Ethyl formic ester
Ethyl methanoate

Molecular Formula: $C_3H_6O_2$

Structure:



Chemical Properties

Molecular Weight: 74.08

Physical State: Liquid

Vapor Pressure: 258.48 mm at 25°C

Vapor Density: 2.55

Boiling Point: 54.5°C at 760 mm

Melting Point: -80.5°C

Density: 0.9236 at 20°C/20°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 30% of theoretical after 10 days

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous
Explosion–severe

Ethyl formate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1850 mg/kg	rat	oral
	2070 mg/kg	rabbit	oral
	1100 mg/kg	guinea pig	oral
LD_{Lo}	8000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Irritant to skin and mucous membranes

Narcotic at high concentrations

TC_{Lo}	330 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA: 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Ethylhexanol

CHEMICAL NAME

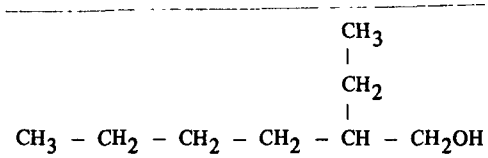
CAS Number: 104-76-7

Chemical Name: 2-Ethyl-1-hexanol

Synonyms: Ethylhexanol
2-Ethylhexyl alcohol
Octyl alcohol

Molecular Formula: $C_8H_{18}O$

Structure:



Chemical Properties

Molecular Weight: 130.23

Physical State: Liquid

Vapor Pressure: 1 mm at 50°C

Vapor Density: 6.35

Boiling Point: 130°C at 50 mm

Melting Point: <-76°C

Density: 0.8859 at 20°C/20°C

Solubility: Slightly (1.16 gm/l H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 86% of theoretical after 20 days at 20°C at 10 mg/ml
Total theoretical oxygen demand = 2.95 gm/gm

Atmospheric Reactivity:
Reacts with oxidizing materials

Safety Hazard: Fire–moderate

PRODUCTION DATA

Annual U.S. Production: 264.7 x 10^6 lbs. (1975)

Consumption: 310.0 x 10^6 lbs. (1975)

Fraction of Dispersion: 0.15

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 79.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3200 mg/kg	rat	oral
	2380 mg/kg	rabbit	skin
LD_{Lo}	3200 mg/kg	mouse	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethylidene chloride

CHEMICAL NAME

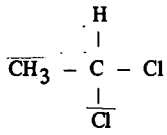
CAS Number: 75-34-3

Chemical Name: 1,1-Dichloroethane

Synonyms: Ethylidene chloride
Ethylidene dichloride
Chlorinated hydrochloric ether

Molecular Formula: $C_2H_4Cl_2$

Structure:



Chemical Properties

Molecular Weight: 98.96

Physical State: Liquid

Vapor Pressure: 230 mm at 25°C

Vapor Density: 3.44

Boiling Point: 57.3°C at 760 mm

Melting Point: -98°C

Density: 1.174 at 20°C/4°C

Solubility: Sparingly (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–dangerous
Explosion–moderate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	725 mg/kg	rat	oral

Non-lethal Acute Effects:
Liver injury

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethyl mercaptan

CHEMICAL NAME

CAS Number: 75-08-1

Chemical Name: Ethanethiol

Synonyms: Ethyl hydrosulfide
Ethyl thioalcohol
Ethyl sulfhydrate

Molecular Formula: C_2H_6S

Structure: $CH_3 - CH_2 - SH$

Chemical Properties

Molecular Weight: 62.13

Physical State: Liquid

Vapor Pressure: 551.91 mm at 25°C

Vapor Density: 2.14

Boiling Point: 35°C at 760 mm

Melting Point: -144.4°C

Density: 0.83907 at 20°C/4°C

Solubility: Slightly soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–dangerous
Explosion–moderate

Ethyl mercaptan

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	682 mg/kg	rat	oral
	450 mg/kg	rat	intraperitoneal
LC_{50}	4420 ppm (4 hours)	rat	inhalation
	2770 ppm	mouse	inhalation

Non-lethal Acute Effects:

CNS irritant			
TC_{Lo}	4 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) Ceiling level: 10 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethyl methanesulfonate

CHEMICAL NAME

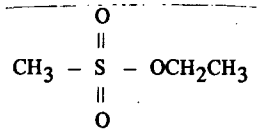
CAS Number: 62-50-0

Chemical Name: Methanesulfonic acid, ethyl ester

Synonyms: Ethyl ester of methylsulfonic acid
Methylsulfonic acid, ethyl ester

Molecular Formula: $C_3H_8O_3S$

Structure:



Chemical Properties

Molecular Weight: 124.17

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 159°C

Melting Point: -37°C

Density: 1.187 at 25°C

Solubility: Very soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Ethyl methanesulfonate

PRODUCTION DATA

Annual U.S. Production: Not produced commercially

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	200 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

TD_{Lo}	36 mg/kg	mouse	parenteral
Neoplasm			
TD_{Lo}	100 mg/kg	rat	intraperitoneal
	83 mg/kg	mouse	subcutaneous

Mutagenicity:

TD_{Lo}	300 mg/kg	rat	intraperitoneal
	380 mg/kg	mouse	intraperitoneal

Teratogenicity:

TLV:

TD_{Lo}	200 mg/kg (13 days)	pregnant rat	intraperitoneal

Other Chronic Effects:

N-Ethylmorpholine

CHEMICAL NAME

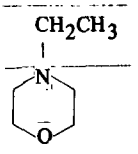
CAS Number: 100-74-3

Chemical Name: 4-Ethylmorpholine

Synonyms: N-Ethylmorpholine

Molecular Formula: $C_6H_{13}NO$

Structure:



Chemical Properties

Molecular Weight: 115.2

Physical State: Liquid

Vapor Pressure:

Vapor Density: 4.00

Boiling Point: 138°C

Melting Point: -63°C

Density: 0.8996 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–moderate

N-Ethylmorpholine

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1780 mg/kg	rat	oral
LC_{Lo}	2000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Irritant to mucous membranes, eyes

TC_{Lo}	100 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 20 ppm (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 20 ppm (skin)

Other Chronic Effects:

Ethyl naphthalene

CHEMICAL NAME

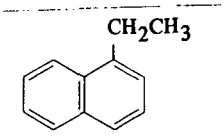
CAS Number: 1127-76-0

Chemical Name: 1-Ethyl naphthalene

Synonyms: Ethyl naphthalene

Molecular Formula: $C_{12}H_{12}$

Structure:



Chemical Properties

Molecular Weight: 156.23

Physical State: Liquid

Vapor Pressure: 1 mm at 20.0°C

Vapor Density:

Boiling Point: 258°C at 760 mm

Melting Point: −13.88°C

Density: 1.0082 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	5000 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethyl oxalate

CHEMICAL NAME

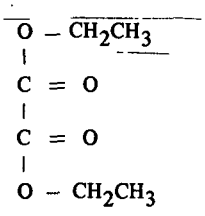
CAS Number: 95-92-1

Chemical Name: Oxalic acid, diethyl ester

Synonyms: Ethyl oxalate
Diethyl oxalate
Diethyl ethaneioate
Oxalic ether

Molecular Formula: $C_6H_{10}O_4$

Structure:



Chemical Properties

Molecular Weight: 146.14

Physical State: Liquid

Vapor Pressure: 1 mm at 47.4°C

Vapor Density: 5.04

Boiling Point: 185.7°C at 760 mm

Melting Point: -38.5°C

Density: 1.0785 at 20°C/4°C

Solubility: Slightly (hot H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate
Disaster hazard–moderate–toxic fumes

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	400 mg/kg	rat	oral

Non-lethal Acute Effects:

Local irritant
Ingestion causes severe damage to kidneys
Caustic effect on mouth, esophogus, and stomach

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethyl parathion

CHEMICAL NAME

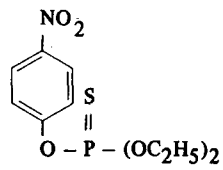
CAS Number: 25737-28-4

Chemical Name: Phosphorothioic acid, O,O-diethyl-O-(p-nitrophenol) ester

Synonyms: Ethyl parathion
O,O-Diethyl O-p-nitrophenyl thiophosphate
Alkron
Compound 3422
Penphos
Vapophor

Molecular Formula: $C_{10}H_{14}NO_3PS$

Structure:



Chemical Properties

Molecular Weight: 291.3

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point: 375°C

Density: 1.26 at 25°C/4°C

Solubility: Slightly soluble (H_2O)

Octanol/Water Partition Coefficient: 2.15

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Ethyl parathion

PRODUCTION DATA

Annual U.S. Production: 15 x 10^6 lbs.

Consumption: 15.0 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 15.2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2 mg/kg	rat	oral
	7 mg/kg	rat	skin
	1500 mg/kg	rat	intraperitoneal
	6 mg/kg	mouse	oral
	40 mg/kg	rabbit	skin
	600 mg/kg	guinea pig	skin
	3 mg/kg	pigeon	oral
	6 mg/kg	quail	oral
	2340 mg/kg	duck	oral
	6 mg/kg	mammal	unreported
	2 mg/kg	wild bird	roal
LC_{Lo}	10 mg/m^3 (2 hours)	rat	inhalation
	50 mg/m^3 (2 hours)	rabbit	inhalation
	14 mg/m^3 (2 hours)	guinea pig	inhalation
LD_{Lo}	240 mg/kg	human	oral
	3 mg/kg	rat	intravenous
	30 mg/kg	mouse	subcutaneous

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 110 $\mu g/m^3$ (skin)

Farm worker field reentry standard

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ethyl silicate

CHEMICAL NAME

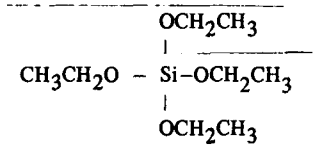
CAS Number: 78-10-4

Chemical Name: Silicic acid, tetraethyl ester

Synonyms: Ethyl silicate
Tetraethyl-o-silicate

Molecular Formula: $C_8H_{20}O_4Si$

Structure:



Chemical Properties

Molecular Weight: 208.30

Physical State: Liquid

Vapor Pressure: 1 mm at 20°C

Vapor Density:

Boiling Point: 168.8°C at 760 mm

Melting Point: -82.5°C

Density: 0.933 at 20°C/4°C

Solubility: Soluble, decomposes (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–moderate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	1000 mg/kg	rat	oral
LC_{Lo}	1000 ppm (4 hours)	rat	inhalation
	1060 ppm (4 hours)	rat	inhalation
	700 ppm (6 hours)	guinea pig	inhalation

Non-lethal Acute Effects:

Irritant to eyes and upper respiratory tract
Nephritis
Liver injury
Anemia
Leucocytosis

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

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15. SUPPLEMENTARY NOTES

16. ABSTRACT

This is the second of a series of four appendices to the report "Scoring of Organic Air Pollutants." The entire appendix contains a compilation of available data on chemical structure and properties, environmental persistence, production, and toxicity for 637 synthetic organic chemicals.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
organic chemical structure organic chemical properties organic chemical production organic chemical toxicity		

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