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PRELIMINARY SCORING OF SELECTED ORGANIC AIR POLLUTANTS APPENDIX IV - CHEMISTRY, PRODUCTION, AND TOXICITY OF CHEMICALS O THROUGH Z

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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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.

TABLE OF CONTENTS

TABLE OF CONTENTS (Continued)

TABLE OF CONTENTS (Continued)

TABLE OF CONTENTS (Concluded)

APPENDIX IV

CHEMISTRY, PRODUCTION AND TOXICITY OF SELECTED SYNTHETIC ORGANIC CHEMICALS

Octyl alcohol

CHEMICAL NAME

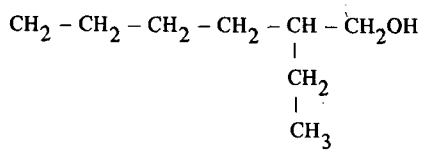
CAS Number: 1341-41-9

Chemical Name: Isooctyl alcohol

Synonyms: 2-Ethylhexyl alcohol
2-Ethyl-l-hexanol

Molecular Formula: $C_8H_{18}O$

Structure:



Chemical Properties

Molecular Weight:	130.23	Physical State:	Liquid
Vapor Pressure:	0.2 mm at 20°C	Vapor Density:	4.49
Boiling Point:	185°C	Melting Point:	-76°C
Density:	0.8328 at 20°C/4°C	Solubility:	Insoluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD: 37% of theoretical

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate

Octyl alcohol

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr): 15.8

TOXICITY DATA

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

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Octyl decyl phthalate

CHEMICAL NAME

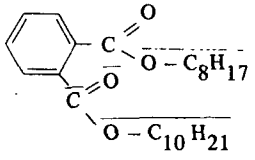
CAS Number: 119-07-3

Chemical Name: Phthalic acid, decyl octyl ester

Synonyms: n-Octyl-n-decyl phthalate
Decyl octyl ester of phthalic acid

Molecular Formula: $C_{26}H_{42}O_4$

Structure:



Chemical Properties

Molecular Weight: 418.6	**Physical State:** Liquid
Vapor Pressure: Negligible at 25°C	**Vapor Density:**
Boiling Point: 239°C at 4 mm	**Melting Point:** −40°C
Density: 0.980 at 20°C/20°C	**Solubility:**
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–slight

Octyl decyl phthalate

PRODUCTION DATA

Annual U.S. Production: 200 x 10^6 lbs.

Consumption: 200 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 203.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Octylphenol

CHEMICAL NAME

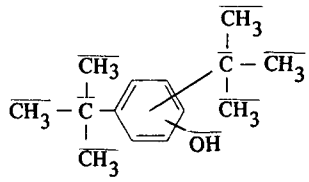
CAS Number: 27193-28-8

Chemical Name: Octylphenol

Synonyms: Diisobutylphenol

Molecular Formula: $C_{14}H_{22}O$

Structure:



Chemical Properties

Molecular Weight: 206.36

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 280 to 283°C

Melting Point:

Density: 0.941 at 24°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–phenol

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}	25 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Oxalic acid

CHEMICAL NAME

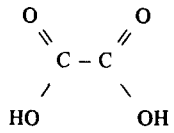
CAS Number: 144-62-7

Chemical Name: Oxalic acid

Synonyms: Ethanedioic acid

Molecular Formula: $C_2H_2O_4$

Structure:



Chemical Properties

Molecular Weight: 90.04

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 150°C (sublimes)

Melting Point: 187°C (anhydrous)

Density: 1.653 (hydrate)

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient: -0.78

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Oxalic acid

PRODUCTION DATA

Annual U.S. Production: 18 x 10^6 lbs. (1974 estimate)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	700 mg/kg	human	oral
	1000 mg/kg	dog	oral

Non-lethal Acute Effects:

Corrosion of mouth, esophagus and stomach
Kidney and liver damage
Irritation of eyes and upper respiratory tract
Corneal damage

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 1 mg/m^3

Other Chronic Effects:

Skin irritation

Paraldehyde

CHEMICAL NAME

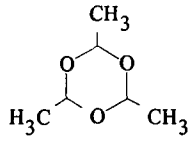
CAS Number: 123-63-7

Chemical Name: 2,4,6-Trimethyl-s-trioxane

Synonyms: Paraldehyde
Para-acetaldehyde

Molecular Formula: $C_6H_{12}O_3$

Structure:



Chemical Properties

Molecular Weight: 132.18

Physical State: Liquid

Vapor Pressure: 25.3 mm at 20°C

Vapor Density: 4.55

Boiling Point: 124.5°C

Melting Point: 12.6°C

Density: 0.9943 at 20°C/4°C

Solubility: Slightly soluble (H_2O)

Octanol/Water Partition Coefficient: 0.95

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous
Explosion–slight

Paraldehyde

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	dog	oral

Non-lethal Acute Effects:

Irritation of eyes and mucous membranes
Dermatitis
Psychotrophic effects

TD_{Lo}	14 mg/kg	human	oral
	14 mg/kg	human	intravenous
	71 mg/kg	human	intramuscular
	14 mg/kg	human	rectal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplasm

TD_{Lo}	12 gm/kg for a week	mouse	skin

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Paraquat

CHEMICAL NAME

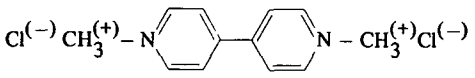
CAS Number: 1910-42-5

Chemical Name: 1,1'-Dimethyl-4,4'-bipyridium dichloride

Synonyms: Paraquat
1,1'-Dimethyl-4,4'-dipyridium salt

Molecular Formula: $C_{12}H_{14}N_2 \cdot 2Cl$

Structure:



Chemical Properties

Molecular Weight: 257.18

Physical State: Solid

Vapor Pressure: non-volatile

Vapor Density:

Boiling Point: Decomposes

Melting Point:

Density: 1.24 to 1.26 at 20°C/20°C

Solubility: Infinite

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Susceptible to ultraviolet decomposition

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: (O, through 1976)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	57 mg/kg	rat	oral
	80 mg/kg	rat	oral
	50 mg/kg	monkey	oral
	22 mg/kg	guinea pig	oral
LD_{Lo}	236 mg/kg	man	oral

Non-lethal Acute Effects:
Lung injury

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TD_{Lo}:	6500 μg/kg (6 days)	pregnant rat	intraperitoneal

TLV:

Other Chronic Effects:

PCNB

CHEMICAL NAME

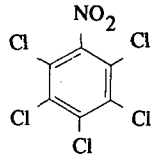
CAS Number: 82-68-8

Chemical Name: Pentachloronitrobenzene

Synonyms: PCNB
Quintozene terrachlor
Tritison

Molecular Formula: $C_6Cl_5NO_2$

Structure:



Chemical Properties

Molecular Weight: 295.32

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 328°C (some decomposition)

Melting Point: 144°C

Density: 1.718 at 25°C/4°C

Solubility: Practically insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard–dangerous–toxic fumes–NO_X and chlorides

PRODUCTION DATA

Annual U.S. Production: 3×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 3.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1650 mg/kg	rat	oral
	1650 mg/kg	mammal	unreported

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

TD_{Lo}	135 gm/kg (77 weeks)	mouse	oral

Neoplastic effects:

TD_{Lo}	576 mg/kg (12 weeks)	mouse	skin

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

PCP

CHEMICAL NAME

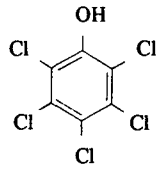
CAS Number: 87-86-5

Chemical Name: Pentachlorophenol

Synonyms: PCP (and salts)

Molecular Formula: C_6HCl_5O

Structure:



Chemical Properties

Molecular Weight: 266.32

Physical State: Solid

Vapor Pressure: 40 mm at 211.2°C

Vapor Density:

Boiling Point: 310°C (decomposes) at 759 mm

Melting Point: 174°C

Density: 1.978 at 22°C/4°C

Solubility: Slightly soluble

Octanol/Water Partition Coefficient: 5.01

Environmental Persistence

BOD:

Atmospheric Reactivity:

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

PRODUCTION DATA

Annual U.S. Production: 46.0 x 10^6 lbs. (1969 capacity)

Consumption: 50.0 x 10^6 lbs. (1975)

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	27 mg/kg	rat	oral
	105 mg/kg	rat	skin
	56 mg/kg	rat	intraperitoneal
	100 mg/kg	rat	subcutaneous
TD_{Lo}	29 mg/kg	human	oral

Non-lethal Acute Effects:

Irritation of skin, eyes, and mucous membranes
Nausea and vomiting

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 500 $\mu g/m^3$

Carcinogenicity:

May be associated with cancer

Mutagenicity:

Mutagen in laboratory

Teratogenicity:

TLV: 500 $\mu g/m^3$

Other Chronic Effects:

Pentaerythritol

CHEMICAL NAME

CAS Number: 115-77-5

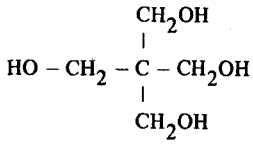
Chemical Name: 2,2-bis(Hydroxymethyl)-1,3-propanediol

Synonyms:

Pentek	PE 200	Pentaerythrite
Penetek		Monopentaerythritol
Tetramethylol		Tetrahydroxymethylmethane

Molecular Formula: $C_5H_{12}O_4$

Structure:



Chemical Properties

Molecular Weight: 136.1

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 276°C at 30 mm (sublimes)

Melting Point: 262°C

Density: 1.399 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–moderate

Pentaerythritol

PRODUCTION DATA

Annual U.S. Production: 100.4 x 10^6 lbs. (1975)

Consumption: 89 x 10^6 lbs. (1975)

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:

Pentane

CHEMICAL NAME

CAS Number: 109-66-0

Chemical Name: Pentane

Synonyms: Amylhydride

Molecular Formula: C_5H_{12}

Structure: $CH_3CH_2CH_2CH_2CH_3$

Chemical Properties

Molecular Weight: 72.15

Physical State: Liquid

Vapor Pressure: 400 mm at 18.5°C

Vapor Density: 2.48

Boiling Point: 36.1°C

Melting Point: −129.72°C

Density: 0.626 at 20°C/4°C

Solubility: Slightly soluble (0.03 gm/100 ml H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–very dangerous
Explosion–severe

PRODUCTION DATA

Annual U.S. Production: 478 x 10^6 lbs. (1964) (all pentanes) **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:			
Narcotic in high concentrations			
CNS effects			
TC_{Lo}	130,000 ppm	human	inhalation
Irritation of eyes and respiratory tract			

Chronic Toxicity

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

Carcinogenicity: Carcinogen

Mutagenicity:

Teratogenicity: **TLV:** 1000 ppm

Other Chronic Effects:

Pentylene

CHEMICAL NAME

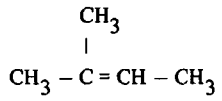
CAS Number: 513-35-9

Chemical Name: 2-Methyl-2-butene

Synonyms: Amylenes (mixed)
Trimethylethylene
3-Methyl-2-butene

Molecular Formula: C_5H_{10}

Structure:



Chemical Properties

Molecular Weight: 70.14

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 38.57°C at 760 mm

Melting Point: -133.77°C

Density: 0.6623 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–dangerous

Pentylene

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:

Moderate effects from ingestion or inhalation

Perchloroethylene

CHEMICAL NAME

CAS Number: 127-18-4

Chemical Name: Tetrachloroethylene

Synonyms: Perchloroethylene
Ethylene tetrachloride
Carbondichloride
Tetrachloroethene

Molecular Formula: C_2Cl_4

Structure:

Chemical Properties

Molecular Weight: 165.82

Physical State: Liquid

Vapor Pressure: 18.47 mm at 25°C

Vapor Density: 5.83

Boiling Point: 121.20°C at 760 mm

Melting Point: -19°C

Density: 1.6227 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Activity: RO_2 $t_{1/2}$ = 220 years
O_3 $t_{1/2}$ = 11 years
OH: $t_{1/2}$ = 8 days

Photochemical Degradation: Not photoreactive

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

Perchloroethylene

PRODUCTION DATA

Annual U.S. Production: 673.7 x 10^6 lbs. (1975)

Consumption: 515 to 575 x 10^6 lbs. (1975 estimate)

Fraction of Dispersion: 0.89

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 688.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	2200 mg/kg	rabbit	subcutaneous
	5000 mg/kg	rabbit	oral
	4000 mg/kg	cat	oral
	85 mg/kg	dog	intravenous
	4000 mg/kg	dog	oral
LC_{Lo}	4000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

TC_{Lo}	600 ppm (10 min)	man–inhalation–central nervous systems effects
	280 ppm (2 hours)	man–inhalation–eye irritant
	230 ppm	human–inhalation–systemic effects

Local irritant; lachrymation; irritation of nose and throat; vomiting, nausea; drowsiness; attitude of irresponsibility; anesthetic; headache; dermatitis; irritation of gastrointestinal tract following ingestion.

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppm
continuous 200 ppm
peak 300 ppm for 5 minutes in 3 hours

Carcinogenicity:
Not carcinogenic according to Dow Chemical Co.

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Perchloromethyl mercaptan

CHEMICAL NAME

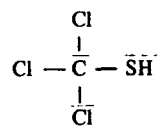
CAS Number: 75-70-7

Chemical Name: Trichloromethanethiol

Synonyms: Perchloromethyl mercaptan Trichloromethyl mercaptan

Molecular Formula: $CHCl_3S$

Structure:



Chemical Properties

Molecular Weight: 151.43

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point:

Density:

Solubility:

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

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

Perchloromethyl 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}	83 mg/kg	rat	oral
LC_{Lo}	483 ppm (10 minutes)	human	inhalation
	58 ppm (10 minutes)	mouse	inhalation
	58 ppm (15 minutes)	cat	inhalation

Non-lethal Acute Effects:

Eye

TC_{Lo}	45 ppm	human	inhalation

Irritation of respiratory tract

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 800 mg/m^3

Carcinogenicity:

Mutagenicity:

TC_{Lo}	15 mg/m^3 (68 weeks)	rat	inhalation

Teratogenicity:

TLV:

Other Chronic Effects:

o-Phenetidine

CHEMICAL NAME

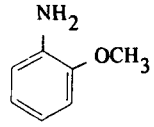
CAS Number: 94-70-2

Chemical Name: o-Phenetidine

Synonyms: 2-Aminophenetole
2-Ethoxyaniline

Molecular Formula: $C_8H_{11}NO$

Structure:



Chemical Properties

Molecular Weight: 137.2

Physical State: Liquid

Vapor Pressure: 1 mm at 67°C

Vapor Density:

Boiling Point: 232.5°C at 760 mm

Melting Point: -20°C

Density:

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard–dangerous–toxic fumes–NO_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**

Sublethal acute effects:

Highly toxic
Palpitation
Dyspnea
Cyanosis

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Recognized carcinogen

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

p-Phenetidine

CHEMICAL NAME

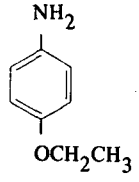
CAS Number: 156-43-4

Chemical Name: p-Phenetidine

Synonyms: 4-Ethoxybenzenamine
4-Aminophenetole
4-Ethoxyaniline

Molecular Formula: $C_8H_{11}NO$

Structure:



Chemical Properties

Molecular Weight: 137.2

Physical State: Liquid

Vapor Pressure: <10 mm at 25°C

Vapor Density: 4.73

Boiling Point: 253 to 255°C

Melting Point: 2 to 4°C

Density: 1.0652 at 16°C/4°C

Solubility: Slightly soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

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

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Recognized carcinogen

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Phenol

CHEMICAL NAME

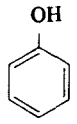
CAS Number: 108-95-2

Chemical Name: Phenol

Synonyms:
Carbolic acid
Phenic acid
Phenylic acid
Oxybenzene
Phenyl hydroxide
Hydroxybenzene

Molecular Formula: C_6H_6O

Structure:



Chemical Properties

Molecular Weight: 94.11

Vapor Pressure: 0.530 mm at 25°C
1 mm at 40°C

Boiling Point: 181.9°C at 760 mm

Density: 1.0576 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density: 3.24

Melting Point: 42.5 to 43°C

Solubility: Soluble (86.6 gm/l H_2O)
Infinitely soluble in hot H_2O

Environmental Persistence

BOD: 96% of theoretical after 20 days at 20°C
Total theoretical oxygen demand = 2.4 gm/gm

Atmospheric Reactivity:

Activity: reacts with oxidizing materials
RO_2 $t_{1/2}$ = 5 mos.
O_3 $t_{1/2}$ = 9.6 hours
OH $t_{1/2}$ = 1 day

Is rapidly biodegraded to catechol, CH_2, CH_3 and –keto–adipate

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

PRODUCTION DATA

Annual U.S. Production: 2,399 x 10^6 lbs. (1974)

Consumption: 2,300 x 10^6 lbs. (1974 estimate)

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 47.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	414 mg/kg	rat	oral
	669 mg/kg	rat	skin
	250 mg/kg	rat	intraperitoneal
	344 mg/kg	mouse	subcutaneous
	300 mg/kg	mouse	oral
LD_{Lo}	140 mg/kg	human	oral
	650 mg/kg	rat	subcutaneous
	80 mg/kg	cat	subcutaneous
	50 mg/kg	cat	intravenous
	420 mg/kg	rabbit	oral
	2000 mg/kg	rabbit	skin
	620 mg/kg	rabbit	intraperitoneal
	620 mg/kg	rabbit	subcutaneous
	180 mg/kg	rabbit	intravenous
	300 mg/kg	guinea pig	intraperitoneal
	450 mg/kg	guinea pig	subcutaneous
	290 mg/kg	frog	parenteral

Non-lethal Acute Effects:

Gastrointestinal Liver and kidney damage Convulsions Estrous cycle disturbances Decreased brain cortex activity	14 mg/kg	human	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: TD_{Lo} 4000 mg/kg (20 weeks) — mouse — skin

Mutagenicity:

Teratogenicity:

TLV: 5 ppm

Other Chronic Effects: Nausea and vomiting
Paralysis

Phenothiazine

CHEMICAL NAME

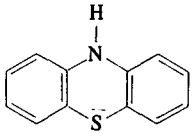
CAS Number: 92-84-2

Chemical Name: Phenothiazine

Synonyms: Thiodiphenylamine
Dibenzo-1,4-thiazine

Molecular Formula: $C_{12}H_9NS$(tricyclic)

Structure:



Chemical Properties

Molecular Weight: 199.3

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 371°C at 760 mm

Melting Point: 185.5 to 185.9°C

Density:

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient: 4.15

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}	5 gm/kg	rat	oral

Non-lethal Acute Effects:

Hemolytic anemia
Toxic degeneration of liver
Skin irritation and photosensitization

TD_{Lo}	425 mg/kg (5 days)	child	oral

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 5 mg/m^3

Other Chronic Effects:

o-Phenylenediamine

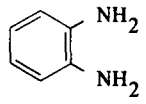
CHEMICAL NAME

CAS Number: 95-54-5

Chemical Name: o-Phenylenediamine

Synonyms: o-Diaminobenzene
1,2-Diamobenzene

Molecular Formula: $C_6H_8N_2$

Structure: 

Chemical Properties

Molecular Weight: 108.1

Physical State: Solid

Vapor Pressure: Negligible

Vapor Density:

Boiling Point: 257°C at 760 mm

Melting Point: 102 to 103°C

Density:

Solubility: Soluble (hot H_2O)

Octanol/Water Partition Coefficient: 0.37

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–slight

o-Phenylenediamine

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}	600 mg/kg	rat	subcutaneous
	600 mg/kg	mouse	subcutaneous

Non-lethal Acute Effects:

Skin and eye irritant
Liver damage

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 $\mu g/m^3$ (skin)

Other Chronic Effects:

p-Phenylenediamine

CHEMICAL NAME

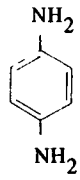
CAS Number: 106-50-3

Chemical Name: p-Phenylenediamine

Synonyms: 1,4-Diaminobenzene
Ursol D

Molecular Formula: $C_6H_8N_2$

Structure:



Chemical Properties

Molecular Weight: 108.16

Physical State: Solid

Vapor Pressure: 1 mm at 98.8°C

Vapor Density: 3.72

Boiling Point: 267°C

Melting Point: 140°C

Density: 1.0696 at 58°C/4°C

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

Octanol/Water Partition Coefficient: -0.26

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Disaster hazard–dangerous toxic fumes

PRODUCTION DATA

Annual U.S. Production: 48×10^6 lbs.

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	100 mg/kg	rat	oral
	50 mg/kg	rat	intraperitoneal
	170 mg/kg	rat	subcutaneous
	100 mg/kg	dog	subcutaneous
	17 mg/kg	dog	intravenous
	100 mg/kg	cat	oral
	100 mg/kg	rabbit	oral
	200 mg/kg	rabbit	subcutaneous
	17 mg/kg	mammal	intravenous

Non-lethal Acute Effects:

Severe skin and eye irritant
Liver damage
Asthma

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

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

Other Chronic Effects:

Phenylhydrazine

CHEMICAL NAME

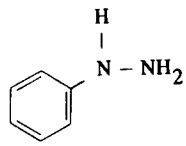
CAS Number: 100-63-0

Chemical Name: Phenylhydrazine

Synonyms: Hydrazinobenzene

Molecular Formula: $C_6H_8N_2$

Structure:



Chemical Properties

Molecular Weight: 108.14

Vapor Pressure: 1 mm at 71.8°C

Boiling Point: 243.5°C at 760 mm

Density: 1.0978 at 20°C/4°C

Octanol/Water Partition Coefficient: 1.25

Physical State: Solid

Vapor Density: 3.7

Melting Point: 19.35°C

Solubility: Very slightly soluble (H_2O)
Soluble in hot H_2O

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Phenylhydrazine

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}	188 mg/kg	rat	oral
	80 mg/kg	rabbit	oral
	80 mg/kg	guinea pig	oral
LD_{Lo}	40 mg/kg	rat	subcutaneous
	175 mg/kg	mouse	oral
	170 mg/kg	mouse	subcutaneous
	200 mg/kg	dog	oral
	120 mg/kg	dog	intravenous
	80 mg/kg	rabbit	subcutaneous
	300 mg/kg	frog	unknown

Non-lethal Acute Effects:

Hemolysis of red blood cells
Gastrointestinal disturbances
Dermatitis
Nausea and vomiting

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 5 ppm

Other Chronic Effects: Damage to kidney and liver
Dermatitis

Phosgene

CHEMICAL NAME

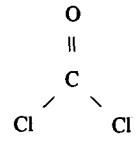
CAS Number: 75-44-5

Chemical Name: Phosgene

Synonyms: Carbonoxychloride
Carbonylchloride
CG

Molecular Formula: CCl_2O

Structure:



Chemical Properties

Molecular Weight: 98.92

Physical State: Gas or volatile liquid

Vapor Pressure: 1428 mm at 25°C

Vapor Density: 3.4

Boiling Point: 7.56°C at 760 mm

Melting Point: -118°C

Density: 1.392 at 19°C/4°C

Solubility: Decomposes in H_2O

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard–highly dangerous–toxic fumes

Phosgene

PRODUCTION DATA

Annual U.S. Production: 728.2 x 10^6 lbs. (1973)

Consumption: 1,066 x 10^6 lbs. (1973)

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LC_{50}	75 ppm (30 months)	rat	inhalation
	110 ppm (30 months)	mouse	inhalation
	1087 ppm (1 month)	monkey	inhalation
	1482 ppm (1 month)	cat	inhalation
	3211 ppm (1 month)	rabbit	inhalation
	141 ppm (30 months)	guinea pig	inhalation
LC_{Lo}	79 ppm (30 months)	dog	inhalation
LD_{Lo}	31 mg/m^3 (20 months)	guinea pig	inhalation
Irritant	25 ppm (30 months)	human	inhalation

Non-lethal Acute Effects:

Corneal opacity
Nausea

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 0.1 ppm

Other Chronic Effects: Pulmonary edema

Phthalic anhydride

CHEMICAL NAME

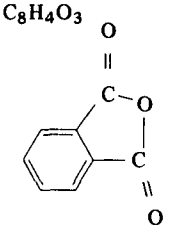
CAS Number: 85-44-9

Chemical Name: Phthalic anhydride

Synonyms: Phalandione

Molecular Formula: $C_8H_4O_3$

Structure:



Chemical Properties

Molecular Weight: 148.12

Physical State: Solid

Vapor Pressure: 1 mm at 96.5°C

Vapor Density: 5.10

Boiling Point: 295.1°C

Melting Point: 131.61°C

Density: 1.527 at 4°C

Solubility: Soluble slightly (hot H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: (Common air contaminant)
Reacts with oxidizing materials

Safety Hazard: Explosion–moderate

Phthalic anhydride

PRODUCTION DATA

Annual U.S. Production: 933 x 10^6 lbs. (703.7 x 10^6 lbs. in 1975)

Consumption: 933.7 x 10^6 lbs.

Fraction of Dispersion: 0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 14.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	4020 mg/kg	rat	oral
	800 mg/kg	guinea pig	oral
LD_{Lo}	100 mg/kg	rat	oral

Non-lethal Acute Effects:
Conjunctivitis

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 2 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 2 ppm

Other Chronic Effects: Emphysema and asthma

Phthalimide

CHEMICAL NAME

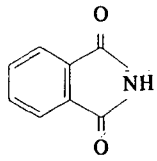
CAS Number: 85-41-6

Chemical Name: 1H-Isoindole-1,3(2H)-dione

Synonyms: Phthalimide
1,3-Isoindoledione
Phthalic acid, imide
Benzoimide

Molecular Formula: $C_8H_5NO_2$

Structure:



Chemical Properties

Molecular Weight: 147.14

Physical State: Solid

Vapor Pressure: < 10 mm at 25°C

Vapor Density:

Boiling Point: 238°C (sublimes)

Melting Point: 238°C

Density:

Solubility: Slightly soluble (H_2O)

Octanol/Water Partition Coefficient: 1.69

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard–slight–toxic fumes

Phthalimide

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:

Phthalonitrile

CHEMICAL NAME

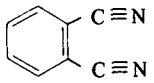
CAS Number: 91-15-6

Chemical Name: Phthalonitrile

Synonyms: o-Dicyanobenzene
1,2-Benzene dicarbonitrile

Molecular Formula: $C_8H_4N_2$

Structure:



Chemical Properties

Molecular Weight: 128.14

Physical State: Solid

Vapor Pressure:

Vapor Density: 4.42

Boiling Point: 187°C (sublimes)

Melting Point: 141°C

Density:

Solubility: Slightly soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard–dangerous–cyanides

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}	1860 mg/kg	rat	oral
	62 mg/kg	rat	intraperitoneal
	65 mg/kg	mouse	oral
	35 mg/kg	mouse	intraperitoneal
	46 mg/kg	mouse	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Picloram

CHEMICAL NAME

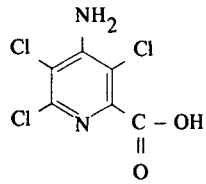
CAS Number: 1918-02-1

Chemical Name: 4-Amino-3,5,6-trichloropicolinic acid

Synonyms: Picloram

Molecular Formula: $C_6H_3Cl_3N_2O_2$

Structure:



Chemical Properties

Molecular Weight: 214.46

Physical State: Solid

Vapor Pressure: 6.16×10^{-7} mm at 35°C

Vapor Density:

Boiling Point: 215°C (decomposes)

Melting Point: 209.5 to 210°C (decomposes at 215°C)

Density:

Solubility: Soluble (H_2O) (430 ppm at 25°C)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Photo decomposition

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}	3750 mg/kg	rat	oral
	1500 mg/kg	mouse	oral
	2000 mg/kg	rabbit	oral
	2000 mg/kg	mammal	unknown

Low toxicity to humans

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

B-Picoline

CHEMICAL NAME

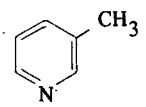
CAS Number: 108-99-6

Chemical Name: 3-Picoline

Synonyms: β-Picoline
3-Methylpyridine

Molecular Formula: C_6H_7N

Structure:



Chemical Properties

Molecular Weight: 93.12

Physical State: Liquid

Vapor Pressure: 10.46 mm at 25°C

Vapor Density: 3.71

Boiling Point: 144.1°C at 760 mm

Melting Point: -18.3°C

Density: 0.9566 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

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

B-Picoline

PRODUCTION DATA

Annual U.S. Production: >60 x 10^6 lbs. (1976)

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:

a, B-Pinene

CHEMICAL NAME

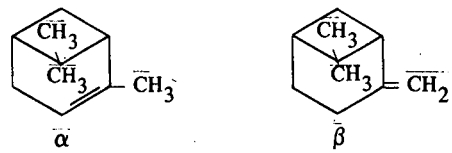
CAS Number: α: 80-56-8 β: 5947-71-7

Chemical Name: α: 2,6,6-Trimethylbicyclo (3.1.1) hept-2-ene
β: 2,6,6-Trimethylbicyclo (3.1.1) hept-1-ene

Synonyms: α: 2-Pinene β: 3-Pinene
Nopinene
Pseudopinene

Molecular Formula: $C_{10}H_{16}$

Structure:



Chemical Properties

Molecular Weight: 136.24

Physical State: Liquid

Vapor Pressure: 1 mm at 37.3°C (unspecified isomer)

Vapor Density: 4.7 (unspecified isomer)

Boiling Point: α: 156.1°C at 760 mm
β: 164 to 166°C at 760 mm

Melting Point: α: −55°C

Density: α: 0.8582 at 20°C/4°C
β: 0.8654 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

PRODUCTION DATA

Annual U.S. Production: 120.7 x 10^6 lbs. (1968) (isomer not specified)

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:

Irritant to skin and mucous membranes
Nephritis

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Piperazine

CHEMICAL NAME

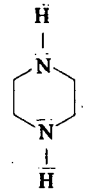
CAS Number: 110-85-0

Chemical Name: Piperazine

Synonyms: Hexahydropyrazine
Dimethylenediamine

Molecular Formula: $C_4H_{10}N_2$

Structure:



Chemical Properties

Molecular Weight: 86.14

Physical State: Solid

Vapor Pressure:

Vapor Density: 3.0

Boiling Point: 146°C at 760 mm

Melting Point: 106°C

Density: 1.1

Solubility: Very soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

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

Piperazine

PRODUCTION DATA

Annual U.S. Production: 4.6×10^6 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}	1100 mg/kg	mouse	subcutaneous

Non-lethal Acute Effects:

Irritant to skin
Blurred vision

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Piperonyl butoxide

CHEMICAL NAME

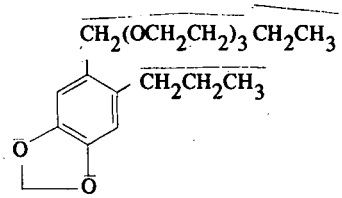
CAS Number: 51-03-6

Chemical Name: α-[2-(2-Butoxyethoxy) ethoxy] -4,5-(methylenedioxy)-2-propyltoluene

Synonyms: Piperonyl butoxide
Butylcarbityl (6-propylpiperonyl) ether
Butacide

Molecular Formula: $C_{19}H_{30}O_5$

Structure:



Chemical Properties

Molecular Weight: 338.4

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 180°C at 1 mm

Melting Point:

Density: 1.04 to 1.07 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

Piperonyl butoxide

PRODUCTION DATA

Annual U.S. Production: 1.0×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated at 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 1.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	11500 mg/kg	rat	oral
	3800 mg/kg	mouse	oral
	7500 mg/kg	rabbit	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Planavin

CHEMICAL NAME

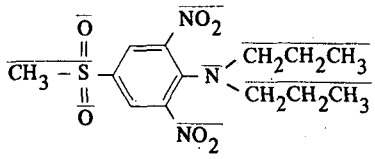
CAS Number: 4726-14-1

Chemical Name: 4-(Methyl sulfonyl)-2,6-dinitro-N,N-dipropylaniline

Synonyms: Planavin

Molecular Formula: $C_{13}H_{19}N_3O_6S$

Structure:



Chemical Properties

Molecular Weight: 345.41	Physical State: Solid or liquid
Vapor Pressure:	Vapor Density:
Boiling Point:	Melting Point: 151 to 152°C
Density:	Solubility:
Octanol/Water Partition Coefficient:	

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 2.0

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}	2000 mg/kg	rat	oral
	2000 mg/kg	mammal	unreported

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Polyacrylamide

CHEMICAL NAME

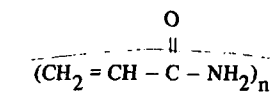
CAS Number: 9005-05-8

Chemical Name: 2-Propenamide, homopolymer

Synonyms: Polyacrylamide
Acrylamide, polymers

Molecular Formula: $(C_3H_5NO)_n$

Structure:



Chemical Properties

Molecular Weight: $(71.08)_n$

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point:

Density:

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Polyacrylamide

PRODUCTION DATA

Annual U.S. Production: 12.8×10^6 lbs.

Consumption: 12.8×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 13.2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Polybutenes

CHEMICAL NAME

CAS Number: 9003-29-6

Chemical Name: Butene, homopolymers

Synonyms: Polybutenes
Butene polymers

Molecular Formula: $(C_4H_8)_n$

Structure: Any of several thermoplastic isotactic polymers of isobutane of varying molecular weight; also polymers of butene-1 and butene-2.

Chemical Properties

Molecular Weight: <3000

Physical State: Liquid

Vapor Pressure: Negligible at 25°C

Vapor Density:

Boiling Point:

Melting Point: -50 to -38°C

Density: 0.83 to 0.89

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Polybutenes

PRODUCTION DATA

Annual U.S. Production: 335.0 x 10^6 lbs. (M.W. <3000)

Consumption: 335.0 x 10^6 lbs.

Fraction of Dispersion: 0.98

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 333.3

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Polychlorinated biphenyl

CHEMICAL NAME

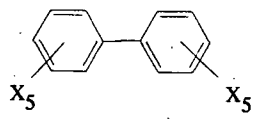
CAS Number: (a) 11097-69-1 (b) 11096-82-5

Chemical Name: (a) Aroclor 1254 (b) Aroclor 1260

Synonyms: (a) PCB 1254
Chlorinated biphenyls
Polychlorinated biphenyls
(b) PCB 1260
Kanechlor

Molecular Formula: (exact composition unknown or undetermined)

Structure:



X = Cl or H

Chemical Properties (Aroclor 1254)

Molecular Weight:

Physical State: Liquid–solid

Vapor Pressure: <1 mm at 25°C

Vapor Density:

Boiling Point: 365 to 390°C

Melting Point:

Density: 1.495 to 1.505 at 65°C/15.5°C

Solubility: Slight (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Activity towards OH: $t_{1/2}$ = 26 days

Safety Hazard:

Disaster hazard–dangerous–toxic fumes

PRODUCTION DATA

Annual U.S. Production: 5.495 x 10^6 lbs.

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 30.3

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Non-lethal Acute Effects:
Liver damage

Chronic Toxicity

U.S. Occupational Standard: **Aroclor 1254 - 0.5 mg/m^3**
Aroclor 1242 - 1.0 mg/m^3

Carcinogenicity:

Kanechlor 500			
Neoplasm			
TD_{Lo}	17 gm/kg (49 weeks)	rat	oral
Carcinogenicity	23 gm/kg (32 weeks)	mouse	oral
Kanechlor 400			
Neoplasm	7500 mg/kg (1.5 years)	rat	oral
Skin effects			
TD_{Lo}	28 mg/kg	human	oral
Kanechlor 300			
Neoplasm			
TD_{Lo}	18 gm/kg (52 weeks)	rat	oral

Mutagenicity:

Teratogenicity:

Other Chronic Effects:

Polyethylene and co-polymers

CHEMICAL NAME

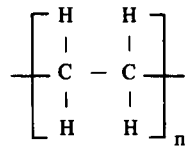
CAS Number: 9002-88-4

Chemical Name: Ethylene, polymers

Synonyms: Polyethylene

Molecular Formula: $(C_2H_4)_n$

Structure:



(chain is linear)

Chemical Properties

Molecular Weight: $(28.05)_n$

Physical State: Solid

Vapor Pressure: Negligible mm at 25°C

Vapor Density:

Boiling Point: 85 to 110°C

Melting Point: 85 to 110°C

Density: 0.92 average

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Polyethylene and co-polymers

PRODUCTION DATA

Annual U.S. Production: 2295.9 x 10^6 lbs.

Consumption: 2010.8 x 10^6 lbs.
1975: High density polymers–2,289 x 10^6 lbs.
Low density polymers–4,725 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 2079.7

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplasm			
TD_{Lo}	2120 mg/kg	rat	implant
	330 mg/kg	mouse	implant

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Polyethylene glycol

CHEMICAL NAME

CAS Number: 25322-68-3

Chemical Name: Polyethylene glycols

Synonyms: Polyoxyethylene
Polyglycol
Ethylene oxide polymer
Polyglycol ether

Molecular Formula: $(C_2H_4O)_nH_2O$

Structure: $H(OCH_2CH_2)_nOH$

Chemical Properties

Molecular Weight: 200 to 6000

Physical State: Liquid

Vapor Pressure: Negligible to 25°C

Vapor Density:

Boiling Point:

Melting Point: 4 to 10°C

Density: 1.110 to 1.140 at 20°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 5% of theoretical after 10 days at 20°C with acclimated culture
Total theoretical oxygen demand = 1.7 (gm/gm)

Atmospheric Reactivity:

Safety Hazard:
Fire–moderate

Polyethylene glycol

PRODUCTION DATA

Annual U.S. Production: 52.4×10^6 lbs.

Consumption: 44.4×10^6 lbs.

Fraction of Dispersion: 0.70

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 31.8

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: TD_{Lo}	420 mg/kg (1 year)	mouse	intravaginal

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Polyethylene glycol chloride

CHEMICAL NAME

CAS Number: (Not listed in 9th Chemical Index)

Chemical Name:

Synonyms: Poly(ethylene glycol) chloride

Molecular Formula: $(C_2H_9O)_nHCl$

Structure: $Cl(CH_2 - CH_2 - O)_nH$

Chemical Properties

Molecular Weight: 100 to 600

Physical State: Liquid

Vapor Pressure: (low)

Vapor Density: 4.31

Boiling Point:

Melting Point: -90°C to 20°C (sets)

Density: 1.18 to 1.14 at 20°C/20°C

Solubility: Miscible (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

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

Polyethylene glycol 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
LD_{50}	1070 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Polyethylene terephthalate

CHEMICAL NAME

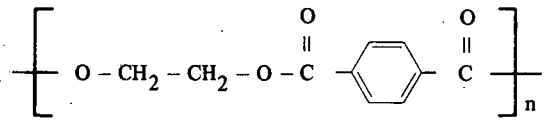
CAS Number: 25038-59-9

Chemical Name: Poly(oxy-1,2-ethanediyloxycarbonyl-1,4-phenylenecarbonyl)

Synonyms: Polyethylene terephthalate
Polyester resin
Poly(oxyethyleneoxyterephthaloyl)

Molecular Formula: $(C_{10}H_8O_4)_n$

Structure:



Chemical Properties

Molecular Weight: $(192.17)_n$

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: Decomposes

Melting Point: 265°C

Density:

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Polyethylene terephthalate

PRODUCTION DATA

Annual U.S. Production: 2500 x 10^6 lbs.

Consumption: 2450 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2487.5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplasm	Dosage	Animal	Route
TD_{Lo}	50 mg/kg	rat	implant

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Polypropylene

CHEMICAL NAME

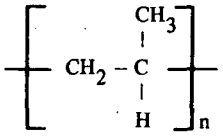
CAS Number: 9003-07-0

Chemical Name: 1-Propene, homopolymer

Synonyms: Polypropylene
Propene, polymers

Molecular Formula: $(C_3H_6)_n$

Structure:



Chemical Properties

Molecular Weight: >40,000 $(42.09)_n$

Physical State: Solid

Vapor Pressure: Negligible at 25°C

Vapor Density:

Boiling Point:

Melting Point: 167°C (isotactic)

Density: 0.90

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Polypropylene

PRODUCTION DATA

Annual U.S. Production: 2,162 x 10^6 lbs. (1973)

Consumption: 1,924 x 10^6 lbs. (1973)

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 1563.2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Polypropylene glycol

CHEMICAL NAME

CAS Number: 25322-69-4

Chemical Name: α-Hydro-O-hydroxypoly [oxy (methyl-1,2-ethanediyl)]

Synonyms: Polypropylene glycols
Poly (propylene oxide)
Polyglycol

Molecular Formula: $(C_3H_6O)_nH_2O$

Structure: $\overline{HO(C_3H_6O)_nH}$

Chemical Properties

Molecular Weight: (76.11-monomer) 400 to 2000

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 189°C (monomer)

Melting Point: Does not crystalize

Density: 1.002 to 1.007

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire-slight

Polypropylene glycol

PRODUCTION DATA

Annual U.S. Production: 359.2 x 10^6 lbs.

Consumption: 302.2 x 10^6 lbs.

Fraction of Dispersion: 0.07

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 26.6

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	419 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Polystyrene

CHEMICAL NAME

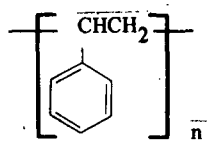
CAS Number: 9003-53-6

Chemical Name: Ethynlbenzene, homopolymer

Synonyms: Styrene, polymers
Polystyrene, straight (thermoplastic resins)
Phenylethylene
Vinylbenzene

Molecular Formula: $(C_8H_8)_n$

Structure:



n = 500-2000

Chemical Properties (monomer)

Molecular Weight: 104.16

Physical State: Solid

Vapor Pressure: Negligible

Vapor Density:

Boiling Point: 145.2°C at 760 mm

Melting Point: -30.63

Density: 0.9060 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: 3,322 x 10^6 lbs. (1973)

Consumption: 3,005 x 10^6 lbs. (1973)
(2,641 x 10^6 lbs., 1975)

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 1471

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplasm			
TD_{Lo}	19 mg/kg	rat	implant

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Polystyrene, thermoplastic resins

CHEMICAL NAME

CAS Number: (Chemical mixture)

Chemical Name:

Synonyms: Polystyrene, rubber modified (thermoplastic resins)
Styrene, polymers

Molecular Formula: $(C_8H_8)_n$

Structure: Mixture of polystyrene and polybutadiene

Chemical Properties

Molecular Weight:

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point:

Density: 1.01 to 1.07

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Polystyrene, thermoplastic resins

PRODUCTION DATA

Annual U.S. Production: 1647 x 10^6 lbs.

Consumption: 1678 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 1,727.4

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Reports of leukemia at rubber plants

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Polytetrafluoroethylene

CHEMICAL NAME

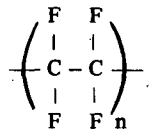
CAS Number: 116-14-3

Chemical Name: Tetrafluoroethene

Synonyms: Teflon
TFE
Perfluoroethylene

Molecular Formula: C_2F_4

Structure:



Chemical Properties (Monomer)

Molecular Weight: 100.02

Physical State: Gas

Vapor Pressure:

Vapor Density:

Boiling Point: -76.3°C at 760 mm

Melting Point: -142.5°C

Density: 1.519 at 76.3°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Resistant to oxidation, moisture, ozone and U.V. radiation

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

Polytetrafluoroethylene

PRODUCTION DATA

Annual U.S. Production: 13.2 x 10^6 lbs.

Consumption: 14.6 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 15.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Non-lethal Acute Effects:
Dust can cause "polymer fume fever"

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:
Neoplasm

TD_{Lo}	80 mg/kg	rat	implant

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Polyvinyl alcohol

CHEMICAL NAME

CAS Number: 9002-89-5

Chemical Name: Ethanol, homopolymer

Synonyms: Polyvinyl alcohol
PVA
Vinyl alcohol, polymers

Molecular Formula: $(C_2H_4O)_n$

Structure: $-\left(CH_2CH\,OH\right)-_n$

Chemical Properties

Molecular Weight: 25,000 to 300,000

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: >200°C (decomposes)

Melting Point:

Density: 1.329

Solubility: Solubility in H_2O increases with increasing molecular weight.

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–slight
Explosion–slight

Polyvinyl alcohol

PRODUCTION DATA

Annual U.S. Production: 100 to 141 x 10^6 lbs. (1974)

Consumption: 141.1 x 10^6 lbs. (1975)

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 104.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

TD_{Lo}	2500 mg/kg	rat	subcutaneous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Polyvinyl chloride

CHEMICAL NAME

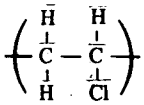
CAS Number: 9002-86-2

Chemical Name: Chloroethylene, polymers

Synonyms: Polyvinyl chloride
PVC

Molecular Formula: $(C_2H_3Cl)_n$

Structure:



Chemical Properties

Molecular Weight: 60,000

Physical State: Solid

Vapor Pressure: Negligible at 25°C

Vapor Density:

Boiling Point: Decomposes

Melting Point:

Density: 1.406

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Photochemical degradation: Biodegradable, photodegradable
Unreactive to RO_2, O_3
Hydrolysis is slow (rates unknown)

Safety Hazard:

Disaster hazard–dangerous–toxic fumes

Polyvinyl chloride

PRODUCTION DATA

Annual U.S. Production: 4,562 x 10^6 lbs. (1973)

Consumption: 4,586 x 10^6 lbs. (1973)
(3,615 x 10^6 lbs. in 1975)

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 4385.7

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
Non-lethal Acute Effects:			
Dermatitis			

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Carcinogen (sarcomas, granulomas)

Neoplasm:			
TD_{Lo}	100 mg/kg	rat	implant
Mutagenicity:			
Teratogenicity:			
Positive		rat	intraperitoneal
		TLV:	

Other Chronic Effects:

Princep

CHEMICAL NAME

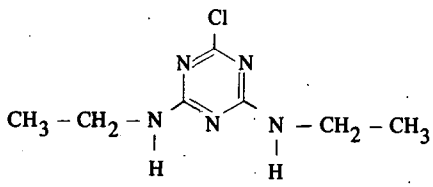
CAS Number: 122-34-9

Chemical Name: 2-Chloro-4,6-bis(ethylamino)-s-triazine

Synonyms: 2-Chloro-4,6-bis(dimethylamino)-s-triazine

Molecular Formula: $C_7H_{12}ClN_5$

Structure:



Chemical Properties

Molecular Weight: 221.75

Physical State: Liquid

Vapor Pressure: 6.1×10^{-9} mm at 20°C

Vapor Density:

Boiling Point:

Melting Point: 225 to 227°C

Density: 1.0956

Solubility: 5 ppm H_2O at 20°C

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Decomposed by ultraviolet irradiation

Safety Hazard:
Disaster hazard–dangerous–chlorides

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}	5000 mg/kg	rat	oral

No toxicity in man reported

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Propachlor

CHEMICAL NAME

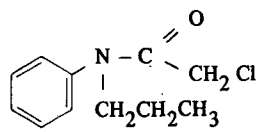
CAS Number: 1918-16-7

Chemical Name: 2-Chloro-N-(1-methylethyl)-N-phenylacetamide

Synonyms: Ramrod
2-Chloro-N-isopropylacetanilide
N-Isopropyl-2-chloroacetanilide

Molecular Formula: $C_{11}H_{14}ClNO$

Structure:



Chemical Properties

Molecular Weight: 211.5

Physical State: Solid

Vapor Pressure: 2.3×10^{-4} mm at 25°C

Vapor Density:

Boiling Point: 110°C at 0.03 mm

Melting Point: 67 to 76°C

Density:

Solubility: 700 ppm (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

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

Propachlor

PRODUCTION DATA

Annual U.S. Production: 23×10^6 lbs.

Consumption: 23×10^6 lbs.

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 23.2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1200 mg/kg	rat	oral
	380 mg/kg	rabbit	skin
	800 mg/kg	mammal	unreported

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Skin and eye irritant

Propane

CHEMICAL NAME

CAS Number: 74-986

Chemical Name: Propane

Synonyms: Dimethyl methane

Molecular Formula: C_3H_8

Structure: $CH_3 - CH_2 - CH_3$

Chemical Properties

Molecular Weight: 44.09

Physical State: Gas

Vapor Pressure: 7095 mm at 25°C

Vapor Density: 1.56

Boiling Point: -42.07°C at 760 mm

Melting Point: -189.9°C

Density: 0.5852 at -44.5°C/4°C

Solubility: 119 gm/l (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts vigorously with oxidizing materials

Safety Hazard:
Fire–highly dangerous
Explosion–severe

Propane

PRODUCTION DATA

Annual U.S. Production: 9608.3 x 10^6 lbs.

Consumption: 9608.3 x 10^6 lbs.

Fraction of Dispersion: 0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 96.1

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Non-lethal Acute Effects:

Paralysis by inhalation of concentrated gas

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 1000 ppm

Other Chronic Effects:

Propanil

CHEMICAL NAME

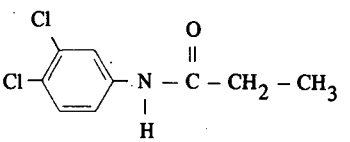
CAS Number: 709-98-8

Chemical Name: N-(3,4-Dichlorophenyl)propanamide

Synonyms: Propanil
3,4-Dichloropropionanilide

Molecular Formula: $C_9H_9Cl_2NO$

Structure:



Chemical Properties

Molecular Weight: 218.09

Physical State: Solid (pure compound)
Liquid (technical compound)

Vapor Pressure:

Vapor Density:

Boiling Point: 91 to 95°C (technical)

Melting Point: 85 to 89°C (pure)

Density: 1.25 at 25°C

Solubility: 0.05% in H_2O

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–chlorides

Propanil

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}	1500 mg/kg	rat	oral
	560 mg/kg	rat	oral
	1300 mg/kg	rat	oral
	1217 mg/kg	dog	oral
	500 mg/kg	rabbit	unreported

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Propargyl alcohol

CHEMICAL NAME

CAS Number: 107-19-7

Chemical Name: 2 Propyn-1-ol

Synonyms: Propiolic alcohol

Molecular Formula: C_3H_4O

Structure: $HC \equiv C - CH_2OH$

Chemical Properties

Molecular Weight: 56.07

Physical State: Volatile liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 113.6°C at 760 mm

Melting Point: –48°C

Density: 0.9715 at 20°C/4°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Propargyl alcohol

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}	0.07 mg/kg	rat	oral
LC_{Lo}	2000 mg/kg	mouse	inhalation

Non-lethal Acute Effects:

CNS depressant
Irritant to skin and mucous membranes

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Propazine

CHEMICAL NAME

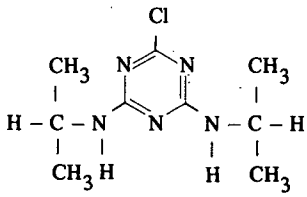
CAS Number: 139-40-2

Chemical Name: 2-Chloro-4,6-bis(isopropylamino)-s-triazine

Synonyms: Propazine

Molecular Formula: $C_9H_{16}ClN_5$

Structure:



Chemical Properties

Molecular Weight: 229.74

Vapor Pressure: 2.9×10^{-8} mm at 20°C

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 212 to 214°C

Solubility: Slightly soluble (8.6 ppm H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Propazine

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}	485 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplasm			
TD_{Lo}	22 gm/kg (82 weeks)	rat	oral
	750 mg/kg (15 weeks)	rat	subcutaneous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Propiolactone

CHEMICAL NAME

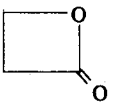
CAS Number: 57-57-8

Chemical Name: 2-Oxetanone

Synonyms: β-Propiolactone
Hydraacrylic acid β lactone
Propanolide
3-Hydroxypropionic acid, lactone

Molecular Formula: $C_3H_4O_2$

Structure:



Chemical Properties

Molecular Weight: 72.06

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 162°C (decomposes)

Melting Point: -33.4°C

Density: 1.1460 at 20°C/5°C

Solubility: Decomposes (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}	345 mg/kg	mouse	intravenous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Carcinogen			
TD_{Lo}	12,865 mg/kg (62 weeks)	hamster	skin
	56,400 mg/kg (141 weeks)	guinea pigs	skin
	3500 mg/kg (70 weeks)	rat	oral
	20 mg/kg (34 weeks)	rat	subcutaneous
	180 mg/kg (30 weeks)	rat	intratracheal
	8100 mg/kg (27 weeks)	mouse	skin
	69 mg/kg (43 weeks)	mouse	subcutaneous
Neoplastic effects:			
TD_{Lo}	40 mg/kg	mouse	intravenous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Propionaldehyde

CHEMICAL NAME

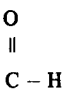
CAS Number: 123-38-6

Chemical Name: Propionaldehyde

Synonyms: Propyl aldehyde
Propylic aldehyde
Propanal
Propionic aldehyde

Molecular Formula: C_3H_6O

Structure:



Chemical Properties

Molecular Weight: 58.08

Physical State: Liquid

Vapor Pressure: 10 mm at 25°C

Vapor Density: 2.0

Boiling Point: 48.8°C

Melting Point: -81°C

Density: 0.8058 at 20°C/4°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient: 0.38

Environmental Persistence

BOD: 95% of theoretical

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous

Propionaldehyde

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}	820 mg/kg	rat	subcutaneous
	680 mg/kg	mouse	subcutaneous
LD_{Lo}	800 mg/kg	rat	oral
	800 mg/kg	mouse	oral
	3400 mg/kg	rabbit	skin
TC_{Lo}	8000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Local irritant to respiratory tract

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Propionic acid

CHEMICAL NAME

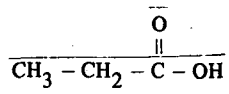
CAS Number: 79-09-4

Chemical Name: Propionic acid

Synonyms: Methylacetic acid
Propanoic acid

Molecular Formula: $C_3H_6O_2$

Structure:



Chemical Properties

Molecular Weight: 74.09

Physical State: Liquid

Vapor Pressure: 4.49 at 25°C

Vapor Density: 2.56

Boiling Point: 141°C at 760 mm

Melting Point: -20.8°C

Density: 0.992

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient: 0.52

Environmental Persistence

BOD: 56% of theoretical

Atmospheric Reactivity:

Safety Hazard: Fire –moderate

Propionic acid

PRODUCTION DATA

Annual U.S. Production: 60.4 x 10^6 lbs. (1973)

Consumption: 60.4 x 10^6 lbs. (1973)
(65 x 10^6 lbs., 1975)

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1510 mg/kg	rat	oral
	1370 mg/kg	mouse	oral
	625 mg/kg	mouse	intravenous
	1900 mg/kg	rabbit	oral
	500 mg/kg	rabbit	skin

Non-lethal Acute Effects:

Local irritant to eyes, skin, and mucous membranes

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Propyl acetate

CHEMICAL NAME

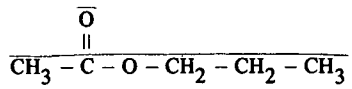
CAS Number: 109-60-4

Chemical Name: Acetic acid, propyl ester

Synonyms: n-Propyl acetate
Propyl ester of acetic acid

Molecular Formula: $C_5H_{10}O_2$

Structure:



Chemical Properties

Molecular Weight:	102.13	Physical State:	Liquid
Vapor Pressure:	40 mm at 28.8°C	Vapor Density:	3.52
Boiling Point:	101.6°C at 760 mm	Melting Point:	−95°C
Density:	0.8898 at 20°C/4°C	Solubility:	Slightly (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD: 72% of theoretical after 20 days at 20°C
Total theoretical oxygen demand = 2.04 gm/gm
Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous
Explosion–moderate

Propyl acetate

PRODUCTION DATA

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

Consumption: 32.4 x 10^6 lbs.

Fraction of Dispersion: 0.75

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 24.8

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	6630 mg/kg	rabbit	oral
LC_{Lo}	8000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Conjunctivitis
Irritation of skin

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 200 ppm

Other Chronic Effects:

Propyl alcohol

CHEMICAL NAME

CAS Number: 71-23-8

Chemical Name: Propyl alcohol

Synonyms: Ethyl carbinol
Propan-1-ol
1-Propanol

Molecular Formula: C_3H_8O

Structure: $\overline{CH_3 - CH_2 - CH_2 - OH}$

Chemical Properties

Molecular Weight: 60.11

Physical State: Liquid

Vapor Pressure: 19.8 mm at 25°C

Vapor Density: 2.07

Boiling Point: 97°C at 760 mm

Melting Point: -126.5°C

Density: 0.8035 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient: 0.74

Environmental Persistence

BOD: 85% of theoretical after 20 days at 20°C
Total theoretical oxygen demand = 2.40 gm/gm

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous
Explosion–moderate

Propyl alcohol

PRODUCTION DATA

Annual U.S. Production: 83.1 x 10^6 lbs.

Consumption: 83.1 x 10^6 lbs.

Fraction of Dispersion: 0.75

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 63.6

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1.9 g/kg	rats	oral
	1870 mg/kg	rats	oral
	3230 mg/kg	mouse	subcutaneous
LD_{Lo}	5700 mg/kg	woman	oral
	140 mg/kg	mouse	oral
	3500 mg/kg	rabbit	oral
	5 mg/kg	mammal	subcutaneous
LC_{Lo}	4000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:
Conjunctivitis
Vomiting
Anemia

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 200 ppm

Other Chronic Effects:

Propylamine

CHEMICAL NAME

CAS Number: 107-10-8

Chemical Name: Propylamine

Synonyms: 1-Aminopropane

Molecular Formula: C_3H_9N

Structure: $\overline{CH_3 - CH_2 - CH_2 - NH_2}$

Chemical Properties

Molecular Weight: 59.11

Physical State: Liquid

Vapor Pressure: 248 mm at 20°C

Vapor Density:

Boiling Point: 47.8°C at 760 mm

Melting Point: -83.0°C

Density: 0.7173 at 20°C/4°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–dangerous

Propylamine

PRODUCTION DATA

Annual U.S. Production: 0.2×10^6 lbs. (1969)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	560 mg/kg	rabbit	skin
LD_{Lo}	570 mg/kg	rat	oral
LC_{50}	2310 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Irritant
Skin sensitizer

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Propyl chloride

CHEMICAL NAME

CAS Number: 540-54-5

Chemical Name: 1-Chloropropane

Synonyms: n-Propylchloride

Molecular Formula: C_3H_7Cl

Structure: $\overline{CH_3 - CH_2 - CH_2 - Cl}$

Chemical Properties

Molecular Weight: 78.54

Physical State: Liquid

Vapor Pressure: 348.8 mm at 25°C

Vapor Density: 2.71

Boiling Point: 46.6°C at 760 mm

Melting Point: -122.8°C

Density: 0.8909 at 20°C/4°C

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous
Explosion–moderate

Propyl 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

Non-lethal Acute Effects:

Irritant to mucous membranes
Narcotic at high concentrations

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Propylene

CHEMICAL NAME

CAS Number: 115-07-1

Chemical Name: Propene

Synonyms: Propylene
Methylethylene

Molecular Formula: C_3H_6

Structure: $\overline{CH_3 - CH = CH_2}$

Chemical Properties

Molecular Weight: 42.09

Physical State: Gas

Vapor Pressure: 8582 mm at 25°C

Vapor Density: 1.46

Boiling Point: -47.4°C at 760 mm

Melting Point: -185.2°C

Density: 0.5139 at 20°C/4°C

Solubility: Slightly (0.78 gm/l H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous
Explosion–moderate

Propylene

PRODUCTION DATA

Annual U.S. Production: 22 to 24 x 10^9 lbs. (1974)

Consumption: 22 to 24 x 10^9 lbs. (1974)

Fraction of Dispersion: 0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 127.1

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
(Mild)			

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Propylene chlorohydrin

CHEMICAL NAME

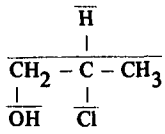
CAS Number: 78-89-7

Chemical Name: 2-Chloro-1-propanol

Synonyms: Propylene chlorohydrin
2-Chloropropyl alcohol

Molecular Formula: C_3H_7ClO

Structure:



Chemical Properties

Molecular Weight: 94.54

Physical State: Liquid

Vapor Pressure: 4.9 mm at 20°C

Vapor Density: 3.26

Boiling Point: 133 to 134°C

Melting Point:

Density: 1.1128 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
Disaster hazard–dangerous–toxic fumes–chlorides

Propylene 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}	220 mg/kg	rat	oral
	480 mg/kg	rabbit	skin
	720 mg/kg	guinea pig	oral
LC_{Lo}	500 mg/kg	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Propylene glycol

CHEMICAL NAME

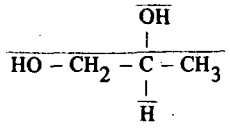
CAS Number: 57-55-6

Chemical Name: 1,2-Propanediol

Synonyms: Propyleneglycol
1,2-Dihydroxy propane

Molecular Formula: $C_3H_8O_2$

Structure:



Chemical Properties

Molecular Weight: 76.11

Physical State: Liquid

Vapor Pressure: 1 mm at 45.5°C

Vapor Density: 2.62

Boiling Point: 187.3°C

Melting Point:

Density: 1.0361 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 79% of theoretical after 20 days at 20°C
Total theoretical oxygen demand = 1.68 gm/gm

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate

Propylene glycol

PRODUCTION DATA

Annual U.S. Production: 562.6 x 10^6 lbs.

Consumption: 454.8 x 10^6 lbs.

Fraction of Dispersion: 0.32

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 154.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	945 mg/kg	rat	oral
	283 mg/kg	rat	intraperitoneal
	195 mg/kg	rat	intravenous
	890 mg/kg	mouse	oral
	471 mg/kg	mouse	intraperitoneal
	285 mg/kg	mouse	subcutaneous
	322 mg/kg	mouse	intravenous
	220 mg/kg	rabbit	intravenous
	821 mg/kg	hamster	oral
	322 mg/kg	hamster	intraperitoneal

Non-lethal Acute Effects:

Local irritant
Allergen

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Propyleneimine

CHEMICAL NAME

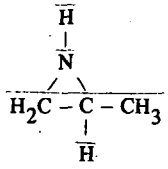
CAS Number: 75-55-8

Chemical Name: 2-Methylaziridine

Synonyms: Propyleneimine
1,2-Propyleneimine

Molecular Formula: C_3H_7N

Structure:



Chemical Properties

Molecular Weight: 58.10

Physical State: Liquid

Vapor Pressure:

Vapor Density: 2.0

Boiling Point: 66 to 67°C

Melting Point:

Density: 0.81 at 25°C/25°C

Solubility: 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–NO_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}	19 mg/kg	rat	oral
	43 mg/kg	guinea pig	skin
LC_{Lo}	500 ppm (4 hours)	rat	inhalation
	500 ppm (1 hour)	guinea pig	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 2 ppm (skin)

Carcinogenicity: Carcinogen

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Propylene oxide

CHEMICAL NAME

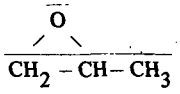
CAS Number: 75-56-9

Chemical Name: Propene oxide

Synonyms: Propylene oxide
Methyl oxirane
1,2-Epoxy propane

Molecular Formula: C_3H_6O

Structure:



Chemical Properties

Molecular Weight: 58.08

Physical State: Liquid

Vapor Pressure: 596 mm at 25°C

Vapor Density: 2.0

Boiling Point: 33.9°C at 760 mm

Melting Point: -104.4°C

Density: 0.8394 at 20°C/4°C

Solubility: Soluble (650 gm/l H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 12% of theoretical after 10 days at 20°C
Total theoretical oxygen demand = 2.2 gm/gm

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–highly dangerous
Explosion–highly dangerous

Propylene oxide

PRODUCTION DATA

Annual U.S. Production: 1640 x 10^6 lbs.

Consumption: 1620 x 10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 40.8

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	930 mg/kg	rat	oral
	1500 mg/kg	rabbit	skin
	690 mg/kg	guinea pig	oral
LC_{50}	1740 ppm (4 hours)	mouse	inhalation
LC_{Lo}	4000 ppm (4 hours)	rat	inhalation
	2005 ppm (4 hours)	dog	inhalation

Chronic Toxicity

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

Carcinogenicity: Experimentation carcinogen

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:
Moderately severe effects from inhalation and ingestion

Pyridine

CHEMICAL NAME

CAS Number: 110-86-1

Chemical Name: Pyridine

Synonyms: Azine
Azabenzene

Molecular Formula: C_5H_5N

Structure:

Chemical Properties

Molecular Weight: 79.10

Physical State: Liquid

Vapor Pressure: 20.3 mm at 25°C

Vapor Density: 2.73

Boiling Point: 115.3°C

Melting Point: –42.0°C

Density: 0.982 at 20°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

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

PRODUCTION DATA

Annual U.S. Production: >60 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
LD_{50}	891 mg/kg	rat	oral
	1000 mg/kg	rat	subcutaneous
	1121 mg/kg	rabbit	skin
LC_{50}	4000 ppm (4 hours)	rat	inhalation
LD_{Lo}	1200 mg/kg	mouse	intraperitoneal
	870 mg/kg	guinea pig	intraperitoneal
	4000 mg/kg	guinea pig	oral

Non-lethal Acute Effects:

Local irritant
CNS depressant
Kidney and liver damage
Gastrointestinal upset

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 5 ppm

Other Chronic Effects:

Randox

CHEMICAL NAME

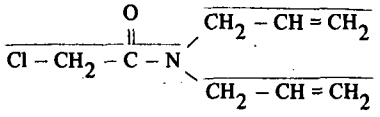
CAS Number: 93-71-0

Chemical Name: N,N-Diallyl-2-chloroacetamide

Synonyms: 2-Chloro-N,N-diallyl acetamide

Molecular Formula: $C_8H_{12}ClNO$

Structure:



Chemical Properties

Molecular Weight:	173.7	Physical State:	Liquid
Vapor Pressure:	<20 mm at 25°C	Vapor Density:	
Boiling Point:	74°C at 0.3 mm	Melting Point:	
Density:		Solubility:	Slightly (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–chlorides

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): 10.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	700 mg/kg	rat	oral
	360 mg/kg	rat	skin
	700 mg/kg	mammal	unreported

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects: Irritant to skin and eyes

Resorcinol

CHEMICAL NAME

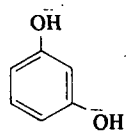
CAS Number: 108-46-3

Chemical Name: Resorcinol

Synonyms: 1,3-Benzendiol
Resorcin
Dihydroxybenzene

Molecular Formula: $C_6H_6O_2$

Structure:



Chemical Properties

Molecular Weight: 110.12

Physical State: Solid

Vapor Pressure: 1 mm at 108.4°C

Vapor Density: 3.79

Boiling Point: 276.5°C at 760 mm

Melting Point: 110.7°C

Density: 1.285 at 15°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient: 0.80

Environmental Persistence

BOD: 61% of theoretical

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–slight

PRODUCTION DATA

Annual U.S. Production: 35 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
LD_{50}	301 mg/kg	rat	oral
	340 mg/kg	mouse	subcutaneous
LD_{Lo}	270 mg/kg	frog	parenteral

Non-lethal Acute Effects:

Dermatitis
Eye irritant
Methemoglobinemia
Convulsions
Tachycardia
Jaundice

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ronnel

CHEMICAL NAME

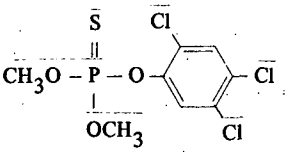
CAS Number: 299-84-3

Chemical Name: Phosphorothioic acid, O,O-dimethyl-O-(2,4,5-trichlorophenyl)ester

Synonyms: Ronnel
Fenchlorphos
O,O-Dimethyl-O-(2,4,5-trichlorophenyl) phosphorothioate

Molecular Formula: $C_8H_8Cl_3O_3PS$

Structure:



Chemical Properties

Molecular Weight: 321.6

Physical State: Solid

Vapor Pressure: 8×10^{-3} mm at 25°C

Vapor Density:

Boiling Point:

Melting Point: 41°C

Density:

Solubility: 800 ppm H_2O

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: 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}	1760 mg/kg	rat	oral
	1000 mg/kg	rabbit	skin
	906 mg/kg	rat	oral
	2000 mg/kg	rat	skin
	2823 mg/kg	rat	intraperitoneal
	118 mg/kg	mouse	intraperitoneal
	80 mg/kg	wild bird	oral
	400 mg/kg	mammal	unreported

Non-lethal Acute Effects:

Edema of lungs
Convulsions
Heart attack
Vomiting

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 15 mg/m^3

Other Chronic Effects:

Ruelene

CHEMICAL NAME

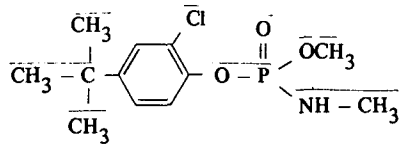
CAS Number: 299-86-5

Chemical Name: Methyl phosphoramidic acid, 4-tert-butyl-2-chlorophenyl methyl ester

Synonyms: Ruelene
4-t-Butyl-2-chlorophenyl-O-methyl methyl phosphoroamidate

Molecular Formula: $C_{12}H_{19}ClNO_3P$

Structure:



Chemical Properties

Molecular Weight: 291.74

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point: 61.8°C

Density: 1.6

Solubility: 0.5 gm/100 ml H_2O at 25°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: 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}	770 mg/kg	rat	oral
	460 mg/kg	rat	oral
	770 mg/kg	rat	unreported
	400 mg/kg	rabbit	oral
	1000 mg/kg	guinea pig	oral
	218 mg/kg	chicken	oral
	100 mg/kg	wild bird	oral

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects: Moderate irritant to eyes
Emesis

Salicylic acid

CHEMICAL NAME

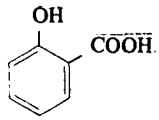
CAS Number: 69-72-7

Chemical Name: Salicylic acid

Synonyms: o-Hydroxybenzoic acid

Molecular Formula: $C_7H_6O_3$

Structure:



Chemical Properties

Molecular Weight: 138.13

Vapor Pressure: 1 mm at 113.7°C

Boiling Point: 211°C at 20 mm (sublimes)

Density: 1.443 at 20°C/4°C

Octanol/Water Partition Coefficient: 2.32

Physical State: Solid

Vapor Density: 4.8

Melting Point: 158 to 161°C

Solubility: Slightly (H_2O)
Very soluble (hot H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Fire–slight
Explosion–slight

PRODUCTION DATA

Annual U.S. Production: 35.0 x 10^6 lbs. (acetosalicate)

Consumption: 35.2 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 35.9

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	891 mg/kg	rat	oral
LD_{60}	520 mg/kg	mouse	subcutaneous
LD_{Lo}	700 mg/kg	rat	subcutaneous
	450 mg/kg	dog	oral
	991 mg/kg	dog	intraperitoneal
	300 mg/kg	dog	subcutaneous
	1300 mg/kg	rabbit	oral
	900 mg/kg	guinea pig	intraperitoneal
	850 mg/kg	guinea pig	subcutaneous
	500 mg/kg	frog	subcutaneous

Non-lethal Acute Effects:

- Nausea
- Rapid pulse
- Skin eruptions

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Silvex

CHEMICAL NAME

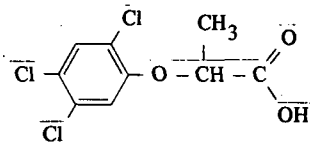
CAS Number: 93-72-1

Chemical Name: 2-(2,4,5-Trichlor-phenoxy)propionic acid

Synonyms: 2,4,5-TCPPA

Molecular Formula: $C_9H_7Cl_3O_3$

Structure:



Chemical Properties

Molecular Weight: 269.5

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point: 180.4 to 181.6°C

Density: 1.640

Solubility: Slightly (140 ppm H_2O at 25°C)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Disaster hazard–dangerous–chlorides

PRODUCTION DATA

Annual U.S. Production: 3×10^6 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}	375-1200 mg/kg	rat	oral
	650 mg/kg	rat	oral
	650 mg/kg	mammal	oral
	650 mg/kg	mammal	unreported

Low toxicity to man

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Sodium acetate

CHEMICAL NAME

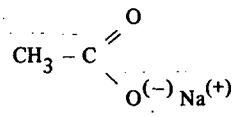
CAS Number: 127-09-3

Chemical Name: Acetic acid, sodium salt

Synonyms:

Molecular Formula: $C_2H_3O_2 \cdot Na$

Structure:



Chemical Properties

Molecular Weight: 83.06

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point: 324°C

Density: 1.528

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 45% of theoretical

Atmospheric Reactivity:

Safety Hazard:

Sodium acetate

PRODUCTION DATA

Annual U.S. Production: 16.5×10^6 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}	3530 mg/kg	rat	oral
	8000 mg/kg	mouse	subcutaneous
	335 mg/kg	mouse	intravenous
LD_{Lo}	3000 mg/kg	dog	intravenous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Sodium benzoate

CHEMICAL NAME

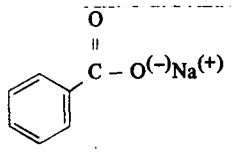
CAS Number: 532-32-1

Chemical Name: Benzoic acid, sodium salt

Synonyms: Benzoate of soda

Molecular Formula: $C_7H_5O_2 \cdot Na$

Structure:



Chemical Properties

Molecular Weight: 144.1

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point:

Density:

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Sodium benzoate

PRODUCTION DATA

Annual U.S. Production: ca. 6 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
LD_{50}	4100 mg/kg	rat	oral
	2000 mg/kg	rabbit	oral
LD_{Lo}	2000 mg/kg	rabbit	subcutaneous
	1400 mg/kg	guinea pig	intraperitoneal
	100 mg/kg	frog	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Sodium carboxymethylcellulose

CHEMICAL NAME

CAS Number: 9004-32-4

Chemical Name: Cellulose, carboxymethyl ether, sodium salt

Synonyms: Sodium carboxymethylcellulose; Cellulose gum; CMC; CM cellulose; Sodium cellulose glycolate

Molecular Formula: (Exact composition unknown or undetermined)

Structure: A synthetic cellulose gum containing 0.4 to 1.5 sodium carboxymethyl group ($-CH_2COO\ Na$) per glucose unit of the cellulose

Chemical Properties

Molecular Weight: ca. 21,000 to 500,000

Physical State: Solid

Vapor Pressure: < 0.6 mm at 25°C

Vapor Density:

Boiling Point: Decomposes

Melting Point:

Density:

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Sodium carboxymethylcellulose

PRODUCTION DATA

Annual U.S. Production: 69.0 x 10^6 lbs.

Consumption: 69.0 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 71.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplasm:

TD_{Lo}	8600 mg/kg (19 weeks)	rat	subcutaneous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Sodium chloroacetate

CHEMICAL NAME

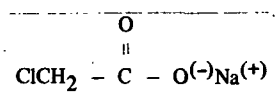
CAS Number: 3926-62-3

Chemical Name: Chloroacetic acid, sodium salt

Synonyms:

Molecular Formula: $C_2H_2ClO_2 \cdot Na$

Structure:



Chemical Properties

Molecular Weight: 116.49

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 200°C (decomposes)

Melting Point:

Density:

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Sodium 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
LD_{50}	76 mg/kg	rat	oral
	165 mg/kg	mouse	oral
	109 mg/kg	mouse	intravenous
	80 mg/kg	guinea pig	oral
LD_{Lo}	100 mg/kg	mammal	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Sodium formate

CHEMICAL NAME

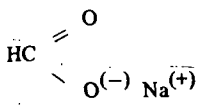
CAS Number: 141-53-7

Chemical Name: Formic acid, sodium salt

Synonyms:

Molecular Formula: $CHO_2 \cdot Na$

Structure:



Chemical Properties

Molecular Weight: 68.01

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 253°C (decomposes)

Melting Point: 253°C

Density: 1.92 at 20°C

Solubility: Soluble (440 gm/l H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 42% of theoretical

Atmospheric Reactivity:

Safety Hazard:
Fire—slight

Sodium formate

PRODUCTION DATA

Annual U.S. Production: 32.0×10^6 lbs.

Consumption: 32.0×10^6 lbs.

Fraction of Dispersion: 0.70

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 22.9

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	807 mg/kg	mouse	intravenous
	2500 mg/kg	mouse	unreported
LD_{Lo}	4000 mg/kg	dog	oral
	3000 mg/kg	dog	intravenous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Sodium phenate

CHEMICAL NAME

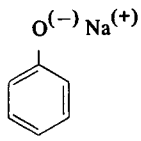
CAS Number: 139-02-6

Chemical Name: Phenol, sodium salt

Synonyms: Sodium phenolate
Sodium carbolate
Sodium phenylate

Molecular Formula: C_6H_5NaO

Structure:



Chemical Properties

Molecular Weight: 116.0

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point:

Density:

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Decomposed by CO_2 of the air

Safety Hazard:

Sodium phenate

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:

Sorbic acid

CHEMICAL NAME

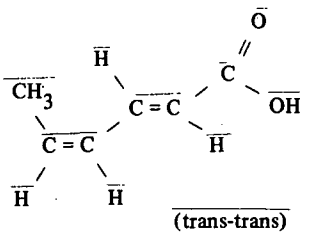
CAS Number: 110-44-1

Chemical Name: Sorbic acid

Synonyms: 2.4-Hexadienoic acid
1,3-Pentadiene-1-carboxylic acid
2-Propenylacrylic acid

Molecular Formula: $C_6H_8O_2$

Structure:



(trans-trans)

Chemical Properties (trans-trans)

Molecular Weight: 112.12

Physical State: Solid

Vapor Pressure: <0.01 mm at 20°C

Vapor Density: 3.87

Boiling Point: 228°C (decomposes)

Melting Point: 134.5°C

Density: 1.204 at 19°C/4°C

Solubility: Soluble (2.5 gm/l H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 70% of theoretical after 10 days at 20°C

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–slight

PRODUCTION DATA

Annual U.S. Production: 40×10^6 lbs.

Consumption: 40×10^6 lbs.

Fraction of Dispersion: 0.50

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 20.6

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	5000 mg/kg	human	unreported
LD_{50}	7400 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

TD_{Lo}	2600 mg/kg (65 weeks)	(rat	subcutaneous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Sorbitol

CHEMICAL NAME

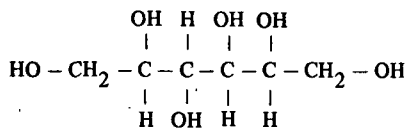
CAS Number: 50-70-4

Chemical Name: D-Glucitol

Synonyms: Hexahydric alcohol
Sorbol

Molecular Formula: $C_6H_{14}O_6$

Structure:



Chemical Properties

Molecular Weight: 182.18

Physical State: Solid

Vapor Pressure: Negligible

Vapor Density:

Boiling Point: 295°C at 3.5 mm

Melting Point: 110 to 112°C (anhydrous)

Density: 1.489 at 20°C/4°C

Solubility: Very soluble (2350 gm/l H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Sorbitol

PRODUCTION DATA

Annual U.S. Production: 84.1 x 10^6 lbs. (1968)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 52.2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Styrene monomer

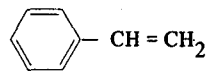
CHEMICAL NAME

CAS Number: 100-42-5

Chemical Name: Styrene

Synonyms: Phenylethylene
Vinyl benzene
Cinnamine

Molecular Formula: C_8H_8

Structure: 

Chemical Properties

Molecular Weight: 104.14

Physical State: Liquid

Vapor Pressure: 6.05 mm at 25°C

Vapor Density:

Boiling Point: 146°C at 760 mm

Melting Point: -30.63°C

Density: 0.9045 at 25°C/25°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 87% of theoretical after 20 days at 20°C
Total theoretical oxygen demand = 3.1 gm/gm

Atmospheric Reactivity: Reacts with oxidizing materials

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

PRODUCTION DATA

Annual U.S. Production: 4394.0 x 10^6 lbs. (1975)

Consumption: 4394.0 x 10^6 lbs.

Fraction of Dispersion: 0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 89.1

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	5000 mg/kg	rat	oral
	216 mg/kg	mouse	oral
LC_{Lo}	10,000 ppm (30 months)	human	inhalation
	5,000 ppm	rat	inhalation
	10,000 ppm	mouse	inhalation
	12 gm/m^3 (14 hours)	guinea pig	inhalation

Non-lethal Acute Effects:

Irritant			
TC_{Lo}	600 ppm	human	inhalation
Central nervous system			
TC_{Lo}	376 ppm	human	inhalation
Glandular			
TC_{Lo}	20 mg/m^3	woman	inhalation

Lachrymation and violent itching of the eyes
Weakness
Stupor
Incoordination
Tremors
Unconsciousness

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppm
Ceiling concentration 200 ppm
Peak concentration 600 ppm/5 minutes/3 hours

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Succinic acid

CHEMICAL NAME

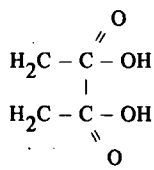
CAS Number: 110-15-6

Chemical Name: Succinic acid

Synonyms: Ethylene succinic acid
Ethylene dicarboxylic acid
Butanedioic acid

Molecular Formula: $C_4H_6O_4$

Structure:



Chemical Properties

Molecular Weight: 118.09

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 235°C (decomposes)

Melting Point: 188°C

Density: 1.564 at 15°C/4°C

Solubility: Slightly (H_2O)
Very soluble (hot 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
LD_{Lo}	2000 mg/kg	frog	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Succinonitrile

CHEMICAL NAME

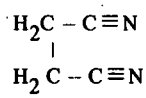
CAS Number: 110-61-2

Chemical Name: Succinonitrile

Synonyms: Butanedinitrile
Ethylenedicyanide

Molecular Formula: $C_4H_4N_2$

Structure:



Chemical Properties

Molecular Weight: 80.09

Physical State: Solid

Vapor Pressure: 2 mm at 100°C

Vapor Density: 270°C

Boiling Point: 267°C at 760 mm

Melting Point: 57 to 57.5°C

Density: 1.022 at 20°C

Solubility: Very soluble (H_2O)

Octanol/Water Partition Coefficient: 0.35

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Disaster hazard–dangerous–toxic fumes of cyanides

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	intraperitoneal
LD_{Lo}	150 mg/kg	dog	unreported
	36 mg/kg	rabbit	unreported
	2200 mg/kg	pigeon	unreported
	1000 mg/kg	frog	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Sulfanilic acid

CHEMICAL NAME

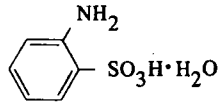
CAS Number: 88-21-1

Chemical Name: o-Aminobenzenesulfonic acid

Synonyms: Sulfanilic acid
Orthanilic acid

Molecular Formula: $C_6H_7NO_3S \cdot H_2O$

Structure:



Chemical Properties

Molecular Weight: 191.2

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point: 288°C (decomposes)

Density: 1.485 at 25°C/4°C

Solubility: Slightly (hot H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–toxic fumes–NO_x and 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**

Non-lethal Acute Effects:
Slight irritation
Low toxicity

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Sulfolane

CHEMICAL NAME

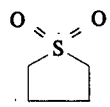
CAS Number: 126-33-0

Chemical Name: Tetrahydrothiophene-1,1-dioxide

Synonyms: Sulfolane
Cyclocyclic tetramethylene sulfone
Cyclo tetramethylene sulfone
Tetramethylene sulfone

Molecular Formula: $C_4H_8O_2S$

Structure:



Chemical Properties

Molecular Weight: 120.18

Physical State: Liquid

Vapor Pressure: 0.01 mm at 20°C

Vapor Density:

Boiling Point: 285°C

Melting Point: 27°C

Density: 1.261 at 30°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Reacts slowly with RO_2 and O_3
Activity toward OH: $t_{1/2}$ = 2 days

Safety Hazard:

PRODUCTION DATA

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

Consumption: 35.0×10^6 lbs.

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 35.5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1540 mg/kg	rat	oral
	1900 mg/kg	mouse	oral
	3180 mg/kg	rabbit	skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Sulfosuccinic, bis(2-ethylhexyl) ester, sodium salt

CHEMICAL NAME

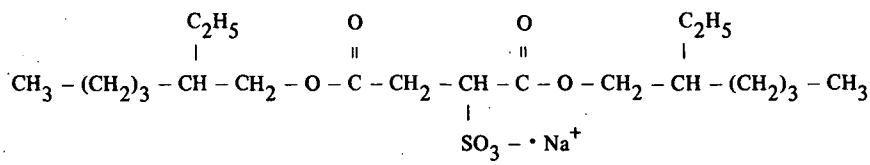
CAS Number: 577-11-7

Chemical Name: Sulfobutanedioic acid,1,4-bis(2-ethylhexyl)ester, sodium salt

Synonyms:

Molecular Formula: $C_{20}H_{37}O_7S \cdot Na$

Structure:



Chemical Properties

Molecular Weight: 445.64

Physical State:

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point:

Density:

Solubility:

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Sulfosuccinic, bis(2-ethylhexyl) ester, sodium salt

PRODUCTION DATA

Annual U.S. Production: 12.4×10^6 lbs.

Consumption: 12.4×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 12.8

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1900 mg/kg	rat	oral
	4800 mg/kg	mouse	oral
	60 mg/kg	mouse	intravenous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Sutan

CHEMICAL NAME

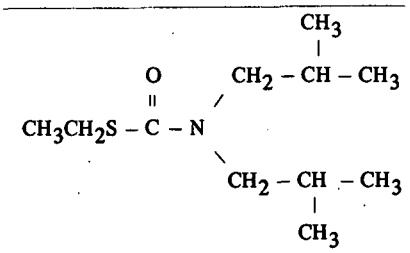
CAS Number: 2008-41-5

Chemical Name: Bis(2-methylpropyl)carbamothioic acid, S-ethyl ester

Synonyms: S-Ethyldiisobutylthiocarbamate

Molecular Formula: $C_{11}H_{23}NOS$

Structure:



Chemical Properties

Molecular Weight: 217.41

Physical State: Liquid

Vapor Pressure: 13×10^{-3} mm at 25°C

Vapor Density:

Boiling Point:

Melting Point:

Density: 0.9402 at 25°C/25°C

Solubility: 45 ppm H_2O at 22°C

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

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}	5366 mg/kg	rat	oral
	4000 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

TBA

CHEMICAL NAME

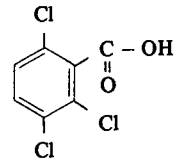
CAS Number: 50-31-7

Chemical Name: 2,3,6-Trichlorobenzoic acid

Synonyms: 2,3,6-TCB
2,3,6-TBA

Molecular Formula: $C_7H_3Cl_3O_2$

Structure:



Chemical Properties

Molecular Weight: 225.46

Vapor Pressure: Negligible

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 124 to 125°C (pure compound)
87 to 99°C (commercial mixture)

Solubility: Slightly soluble (0.84 gm/100 ml H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Relatively stable to ultraviolet decomposition

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}	1644 mg/kg	rat	oral
	650 mg/kg	rat	oral
	1000 mg/kg	rat	intraperitoneal
	615 mg/kg	mouse	oral
	1500 mg/kg	mouse	subcutaneous
	812 mg/kg	rabbit	oral
	1218 mg/kg	guinea pig	oral
	700 mg/kg	mammal	unreported

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

TCA

CHEMICAL NAME

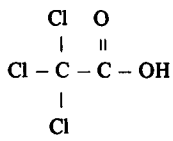
CAS Number: 76-03-9

Chemical Name: Trichloroacetic acid

Synonyms: TCA

Molecular Formula: $C_2HCl_3O_2$

Structure:



Chemical Properties

Molecular Weight: 163.38

Physical State: Solid

Vapor Pressure: 5 mm at 77°C

Vapor Density:

Boiling Point: 197.55°C at 760 mm

Melting Point: 55 to 58°C

Density: 1.62 at 25°C/4°C

Solubility: Very soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 1.0×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 1.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3320 mg/kg	rat	oral
LD_{Lo}	500 mg/kg	mouse	intraperitoneal

Non-lethal Acute Effects:

May cause skin burns upon prolonged contact

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Irritant to nose and throat

Terephthalic acid

CHEMICAL NAME

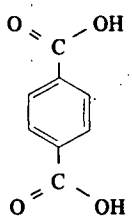
CAS Number: 100-21-0

Chemical Name: Terephthalic acid

Synonyms: p-Phthalic acid
TPA
Benzene-p-dicarboxylic acid

Molecular Formula: $C_8H_6O_4$

Structure:



Chemical Properties

Molecular Weight: 166.14

Physical State: Solid

Vapor Pressure: Negligible

Vapor Density:

Boiling Point: Sublimes

Melting Point: >300° sublimes without melting

Density: 1.51

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Terephthalic acid

PRODUCTION DATA

Annual U.S. Production: 4644.1 x 10^6 lbs. (1975)

Consumption: 4644 x 10^6 lbs.

Fraction of Dispersion: 0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 28.9

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1430 mg/kg	mouse	intraperitoneal
LD_{10}	767 mg/kg	dog	intravenous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Termik

CHEMICAL NAME

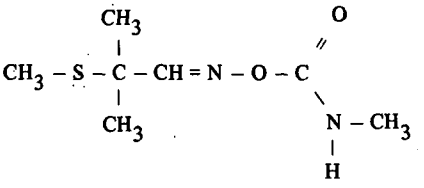
CAS Number: 116-06-3

Chemical Name: 2-Methyl-2(methylthio)propionaldehyde-O-(methyl-carbamoyl)oxime

Synonyms: Termik
Aldicarb

Molecular Formula: $C_7H_{14}N_2O_2S$

Structure:



Chemical Properties

Molecular Weight: 190.1

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point: 100°C

Density:

Solubility:

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: 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}	0.93 mg/kg	rat	oral
	5 mg/kg	rabbit	skin
	1 mg/kg	rat	oral
	2500 µg/kg	rat	skin
	930 µg/kg	rat	unreported
	300 µg/kg	mouse	oral
	1400 mg/kg	rabbit	skin
	4440 µg/kg	duck	oral
LD_{Lo}	666 µg/kg	rat	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

1, 1, 1, 2-Tetrachloro-2, 2-difluoroethane

CHEMICAL NAME

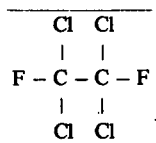
CAS Number: 76-12-0

Chemical Name: 1,1,2,2-Tetrachloro-1,2-difluoroethane

Synonyms: Tetrachlorodifluoroethane

Molecular Formula: $C_2Cl_4F_2$

Structure:



Chemical Properties

Molecular Weight: 203.83

Physical State: Liquid

Vapor Pressure: 52.53 mm at 25°C

Vapor Density: 7.03

Boiling Point: 93°C at 760 mm

Melting Point: 25°C

Density: 1.6447 at 25°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Stable in lower atmosphere

Safety Hazard:
Disaster hazard—dangerous—toxic fumes of chlorides and fluorides

1, 1, 1, 2-Tetrachloro-2, 2-difluoroethane

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}	10,000 ppm (7 hours)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

1, 1, 2, 2-Tetrachloro-1, 2-difluoroethane

CHEMICAL NAME

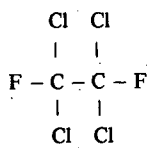
CAS Number: 76-12-0

Chemical Name: 1,1,2,2-Tetrachloro-1,2-difluoroethane

Synonyms: 1,2-Difluoro-1,1,2,2-tetrachloroethane; Freon 112; sym-Tetrachlorodifluoroethane; Genetron 112; F-112

Molecular Formula: $C_2Cl_4F_2$

Structure:



Chemical Properties

Molecular Weight: 208.83

Physical State: Solid or liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 93°C at 760 mm

Melting Point: 25°C

Density: 1.6447 at 25°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Stable in lower atmosphere

Safety Hazard:

1, 1, 2, 2-Tetrachloro-1, 2-difluoroethane

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:

Tetrachloronaphthalene

CHEMICAL NAME

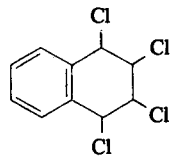
CAS Number: 605-36-7

Chemical Name: 1,2,3,4-Tetrachloro-1,2,3,4-tetrahydronaphthalene

Synonyms:

Molecular Formula: $C_{10}H_8Cl_4$

Structure:



Chemical Properties

Molecular Weight: 269.99

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point: 182°C

Density:

Solubility:

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Disaster hazard–dangerous; when heated to decomposition produces 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
Non-lethal Acute Effects:			
Systemic effects			
TC_{Lo}	3 mg/m^3	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 2 mg/m^3 (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Tetrachlorophthalic anhydride

CHEMICAL NAME

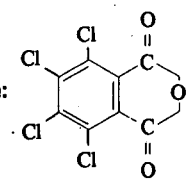
CAS Number: 117-08-8

Chemical Name: Tetrachlorophthalic anhydride

Synonyms:

Molecular Formula: $C_8Cl_4O_3$

Structure:



Chemical Properties

Molecular Weight: 285.90

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 371°C (sublimes)

Melting Point: 255 to 256.5°C

Density:

Solubility: Slightly (decomposes in hot H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Tetrachlorophthalic anhydride

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:

Tetraethyl lead

CHEMICAL NAME

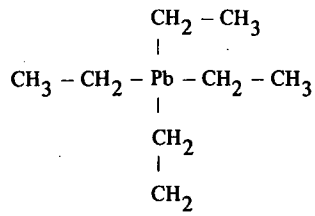
CAS Number: 78-00-2

Chemical Name: Tetraethylplumbane

Synonyms: Tetraethyl lead
TEL

Molecular Formula: $C_8H_{20}Pb$

Structure:



Chemical Properties

Molecular Weight: 323.44

Physical State: Liquid

Vapor Pressure: 1 mm at 28.4°C

Vapor Density:

Boiling Point: 200°C (decomposes)

Melting Point: -136.8°C

Density: 1.659 at 11°C

Solubility: Insoluble (2×10^{-4} g/l H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
With O_3: $t_{1/2}$ = 2-3 days
With RO_2: slow to react in water
With OH: $t_{1/2}$ = 2-3 days

Safety Hazard:
Fire–moderate

PRODUCTION DATA

Annual U.S. Production: 353.0 x 10^6 lbs. (1973)

Consumption: 280.4 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 14.6

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	15 mg/kg	rat	parenteral
LD_{Lo}	17 mg/kg	rat	oral
	10 mg/kg	rat	intraperitoneal
	31 mg/kg	rat	intravenous
	86 mg/kg	mouse	subcutaneous
	500 mg/kg	dog	skin
	23 mg/kg	rabbit	intravenous
	990 mg/kg	guinea pig	skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

TD_{Lo}	86 mg/kg (21 days)	mouse	subcutaneous

Mutagenicity: No information

Teratogenicity: Positive–rat–oral

TLV: 0.0117 mg/m^3

Other Chronic Effects:

Metabolic disturbances
Nervous system disorders
Inhibition of DNA synthesis
Decreased ACHase activity

Tetrahydrofuran

CHEMICAL NAME

CAS Number: 109-99-9

Chemical Name: Tetrahydrofuran

Synonyms:
- Cyclotetramethylene oxide
- 1,4 Epoxy-butone
- Hydrofuron
- Butane α,δ-oxide
- Butylene oxide
- Diethylene oxide
- Oxacyclopentane
- Tetramethylene oxide
- Oxolane
- Furanidine

Molecular Formula: C_4H_8O

Structure:

Chemical Properties

Molecular Weight: 72.10

Physical State: Liquid

Vapor Pressure: 143 mm at 20°C

Vapor Density: 2.5

Boiling Point: 67°C

Melting Point: -65°C

Density: 0.8892 at 20°C/4°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Forms peroxides readily

Safety Hazard:
Fire–dangerous
Explosion–moderate

Tetrahydrofuran

PRODUCTION DATA

Annual U.S. Production: 59.0×10^6 lbs. (90×10^6 lbs., 1975 estimate)

Consumption: 59.0×10^6 lbs.

Fraction of Dispersion: 0.70

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 42.2

TOXICITY DATA

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

Non-lethal Acute Effects:

Narcotic

Irritant to eyes, skin and respiratory tract

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 200 ppm

Other Chronic Effects:

Tetrahydronaphthalene

CHEMICAL NAME

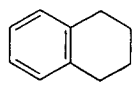
CAS Number: 119-64-2

Chemical Name: 1,2,3,4-Tetrahydronaphthalene

Synonyms: Tetralin

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

Structure:



Chemical Properties

Molecular Weight: 132.21

Physical State: Liquid

Vapor Pressure: 1 mm at 38.0°C

Vapor Density: 4.55

Boiling Point: 207.57°C at 760 mm

Melting Point: -35.79°C

Density: 0.9702 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire—moderate

Tetrahydronaphthalene

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}	2860 mg/kg	rat	oral
LD_{10}	275 ppm (8 hours for 17 days)	guinea pig	inhalation

Non-lethal Acute Effects:

Local irritant
Narcotic in high concentrations

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Cataracts and kidney injury

Tetrahydrophthalic anhydride

CHEMICAL NAME

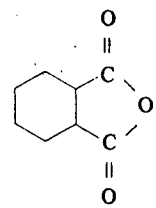
CAS Number: 85-43-8

Chemical Name: 4-Cyclohexene-1,2-dicarboxylic acid

Synonyms: Tetrahydrophthallic anhydride

Molecular Formula: $C_8H_8O_3$

Structure:



Chemical Properties

Molecular Weight:	152.14	Physical State:	Solid
Vapor Pressure:	<0.01 mm at 20°C	Vapor Density:	5.25
Boiling Point:	195°C at 50 mm	Melting Point:	
Density:	1.375 at 25°C/20°C	Solubility:	Insoluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Tetrahydrophthalic anhydride

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}	500 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Tetramethylethylenediamine

CHEMICAL NAME

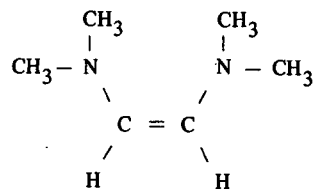
CAS Number: 110-18-9

Chemical Name: N,N,N′,N′-Tetramethylethylenediamine

Synonyms: N,N,N',N'-Tetramethyl-1,2-diaminoethane

Molecular Formula: $C_6H_{16}N_2$

Structure:



Chemical Properties

Molecular Weight: 116.24

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 121 to 122°C

Melting Point: −55.1°C

Density: 0.7765 at 20°C/4°C

Solubility: 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_{Lo}	1580 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Tetramethyl lead

CHEMICAL NAME

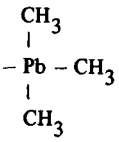
CAS Number: 75-74-1

Chemical Name: Tetramethyl plumbane

Synonyms: Tetramethyl lead
Lead tetramethyl
TML

Molecular Formula: $C_4H_{12}Pb$

Structure:



Chemical Properties

Molecular Weight: 267.33

Physical State: Liquid

Vapor Pressure: 6.0 mm at 10°C

Vapor Density: 9.2

Boiling Point: 110°C at 10 mm

Melting Point: 27.5°C

Density: 1.995

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts vigorously with oxidizing materials

Safety Hazard:
Fire–dangerous
Explosion–moderate

PRODUCTION DATA

Annual U.S. Production: 972.5 x 10^6 lbs. (organo lead compounds)

Consumption: 900 x 10^6 lbs. (organo lead compounds)

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 14.6 (tetramethyl lead)

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	109 mg/kg	rat	oral
	105 mg/kg	rat	parenteral
LD_{Lo}	73 mg/kg	rat	intraperitoneal
	90 mg/kg	rabbit	intravenous

Can be fatal if swallowed

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 90 $\mu g/m^3$ (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 90 $\mu g/m^3$

Other Chronic Effects:

Tetramethyl succinonitrile

CHEMICAL NAME

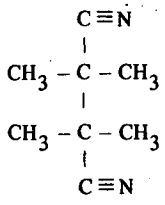
CAS Number: 3333-52-6

Chemical Name: Tetramethyl succinonitrile

Synonyms: TSN

Molecular Formula: $C_8H_{12}N_2$

Structure:



Chemical Properties

Molecular Weight: 136.20

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point: 170.5 to 171.5°C

Density: 1.070

Solubility:

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Tetramethyl succinonitrile

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}	60 ppm	rat	inhalation

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Tetranitromethane

CHEMICAL NAME

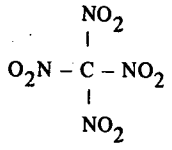
CAS Number: 509-14-8

Chemical Name: Tetranitromethane

Synonyms:

Molecular Formula: CN_4O_8

Structure:



Chemical Properties

Molecular Weight: 196.03

Physical State: Liquid

Vapor Pressure: 1 mm at 22.7°C

Vapor Density:

Boiling Point: 126°C

Melting Point: 14.2°C

Density: 1.6380 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–dangerous
Explosion–severe
Disaster hazard–severe–toxic fumes–NO_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
LC_{Lo}	33 ppm (6 hours)	rat	inhalation
LD_{Lo}	500 mg/kg	mammal	inhalation

Non-lethal Acute Effects:

Irritant to eyes and respiratory passages
Pulmonary edema

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 1 ppm

Other Chronic Effects:

Liver damage
Kidney damage

Tetrapropylene

CHEMICAL NAME

CAS Number: 112-41-4

Chemical Name: 1-Dodecene

Synonyms: α-Dodecylene

Molecular Formula: $C_{12}H_{24}$

Structure: $CH_3(CH_2)_9CH = CH_2$

Chemical Properties

Molecular Weight: 168.33

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 213.4°C at 760 mm

Melting Point: -35.23°C

Density: 0.7584 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Tetrapropylene

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:

Tetryl

CHEMICAL NAME

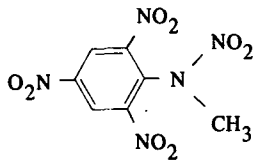
CAS Number: 479-45-8

Chemical Name: N-Methyl-N,2,4,6- tetranitroaniline

Synonyms: Tetryl
Tetralite
Trinitrophenylmethylnitramine
Nitramine

Molecular Formula: $C_7H_5N_5O_8$

Structure:



Chemical Properties

Molecular Weight: 287.15

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: Explodes at 187°C

Melting Point: 131 to 132°C

Density: 1.57 at 19°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–dangerous
Explosion–severe

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	dog	subcutaneous
LD_{Lo}	5000 mg/kg	dog	subcutaneous

Non-lethal Acute Effects:

Dermatitis
Conjunctivitis
Nausea and vomiting

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 1.5 mg/m^3 (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 1.5 mg/m^3 (skin)

Other Chronic Effects:

Anemia
Gastrointestinal conditions

Thiuram

CHEMICAL NAME

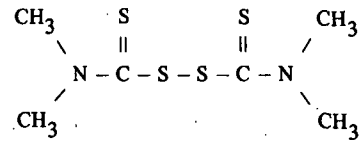
CAS Number: 137-26-8

Chemical Name: Bis(dimethyl thiocarbamoyl)disulfide

Synonyms: Tetramethyl thiuramdisulfide
Disulfuram
TTD
Thiouram

Molecular Formula: $C_6H_{12}N_2S_4$

Structure:



Chemical Properties

Molecular Weight: 240.44

Physical State: Solid

Vapor Pressure: Negligible

Vapor Density:

Boiling Point: 129°C at 20 mm

Melting Point: 155 to 156°C

Density: 1.30 at 20°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–NO_x and SO_x

PRODUCTION DATA

Annual U.S. Production: 15.7×10^6 lbs. (1972)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	560 mg/kg	rat	oral
	1350 mg/kg	mouse	oral
	210 mg/kg	rabbit	oral
	780 mg/kg	mammal	unknown
LD_{Lo}	200 mg/kg	mouse	intraperitoneal
	230 mg/kg	cat	oral

Non-lethal Acute Effects:

Liver and kidney injury
Brain damage
Irritation of eyes, nose and throat

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 5 mg/m^3 (air)

TD_{Lo}	250 mg/kg (6-17 days of pregnancy)	mouse	oral
	250 mg/kg (8 days of pregnancy)	hamster	oral

Other Chronic Effects:

o-Tolidine

CHEMICAL NAME

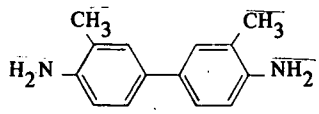
CAS Number: 119-93-7

Chemical Name: 3,3'-Dimethylbenzidine

Synonyms: o-Tolidine
3,3'-Dimethyldiphenyl-4,4'-diamine

Molecular Formula: $C_{14}H_{16}N_2$

Structure:



Chemical Properties

Molecular Weight: 212.30

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point: 131 to 132°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
LD_{50}	404 mg/kg	rat	oral
LD_{Lo}	125 mg/kg	rat	intraperitoneal
	125 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Recognized carcinogen

TD	2250 mg/kg (30 days)	rat	oral
	2880 mg/kg (34 weeks)	rat	subcutaneous
	4480 mg/kg (1 year)	rat	implant

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Toluene

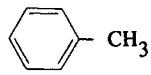
CHEMICAL NAME

CAS Number: 108-88-3

Chemical Name: Toluene

Synonyms: Methyl benzene
Phenyl methane
Toluol

Molecular Formula: C_7H_8

Structure: 

Chemical Properties

Molecular Weight: 92.15

Physical State: Liquid

Vapor Pressure: 28.4 mm at 25°C

Vapor Density: 3.14

Boiling Point: 110.6°C at 760 mm

Melting Point: -95°C

Density: 0.8669 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient: 2.80

Environmental Persistence

BOD: 86% of theoretical after 20 days at 20°C
Total theoretical oxygen demand = 3.13 gm/gm

Atmospheric Reactivity:
Reacts with oxidizing materials
Unreactive to O_3 and RO_2 ($T_{1/2} = 10^3 - 10^6$ days)
Reactive toward OH
No photochemical degradation

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

PRODUCTION DATA

Annual U.S. Production: 6,937.9 x 10^6 lbs. (1974)

Consumption: 5,420 x 10^6 lbs. (1975)

Fraction of Dispersion: 0.15

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 1074.2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	5400 mg/kg	rat	oral
	1640 mg/kg	rat	intraperitoneal
LC_{50}	5300 ppm	mouse	inhalation
LD_{Lo}	800 mg/kg	rat	intraperitoneal
	5000 mg/kg	rat	subcutaneous
LC_{Lo}	4000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Central nervous system			
TC_{Lo}	200 ppm	human	inhalation
Psychotrophic			
TC_{Lo}	100 ppm	man	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) NIOSH Recommended Standard:
- TWA 200 ppm
- Ceiling 300 ppm
- Peak concentration 500 ppm/10 minutes

Carcinogenicity:

(Suspected) 100% solution	mouse	dermal

Mutagenicity:

Teratogenicity:

TLV:
Odor perception: 40 ppm

Other Chronic Effects:
- Blood abnormalties
- Bone marrow chromosome damage
- Metabolic effects
- Enzymatic effects
- Increased liver microsomal enzymes

Toluene-2, 4-diamine

CHEMICAL NAME

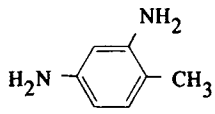
CAS Number: 95-80-7

Chemical Name: Toluene-2,4-diamine

Synonyms: Tolylene diamine
2,4-Diaminotoluene

Molecular Formula: $C_7H_{10}N_2$

Structure:



Chemical Properties

Molecular Weight: 122.17

Physical State: Solid

Vapor Pressure: 1 mm at 106.5°C

Vapor Density:

Boiling Point: 292°C

Melting Point: 99°C

Density:

Solubility: Very soluble (hot H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–moderate–toxic fumes

Toluene-2, 4-diamine

PRODUCTION DATA

Annual U.S. Production: 63×10^6 lbs.

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	500 mg/kg	rat	oral
	50 mg/kg	rat	unreported
	200 mg/kg	dog	subcutaneous
	350 mg/kg	dog	unreported
	400 mg/kg	rabbit	unreported
	200 mg/kg	guinea pig	unreported

Non-lethal Acute Effects:

Liver damage
Skin irritation
Anemia

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplasm:

TD_{Lo}	280 mg/kg (35 weeks)	rat	subcutaneous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Toluene diisocyanate

CHEMICAL NAME

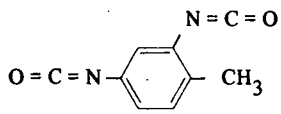
CAS Number: 91-08-7

Chemical Name: Isocyanic acid, 2-methyl-m-phenylene ester

Synonyms: Isocyanic acid, methyl phenylene ester
TDI
2,4-Toluene diisocyanate

Molecular Formula: $C_9H_6N_2O_2$

Structure:



Chemical Properties

Molecular Weight: 174.16

Physical State: Liquid

Vapor Pressure: <0.01 mm at 20°C

Vapor Density: 6.0

Boiling Point: 238.3°C

Melting Point: 19.5 to 21.5°C

Density: 1.22 at 20°C/4°C

Solubility: Reacts with H_2O producing CO_2

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Reacts slowly with O_3 and RO_2
$T_{½}$ OH = 3 days
Hydrolyzes in H_2O (pH 7.0) $t_{½}$ = 0.5 seconds

Safety Hazard:
Disaster hazard–dangerous–toxic fumes

Toluene diisocyanate

PRODUCTION DATA

Annual U.S. Production: 420 x 10^6 lbs.

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 6.3

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LC_{50}	14 ppm (4 hours)	rat	inhalation
	10 ppm (4 hours)	mouse	inhalation
	13 ppm (4 hours)	guinea pig	inhalation

Non-lethal Acute Effects:

Irritant

TC_{Lo}	0.5 ppm	human	inhalation

Pulmonary edema

Allergies produced severe dermatitis and bronchial spasms

Chronic Toxicity

U.S. Occupational Standard: (air) Ceiling–140 $\mu g/m^3$
NIOSH recommends: (air) TWA 5 ppb

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 0.02 ppm–below level of odor perception

Other Chronic Effects:
Liver disease

Toluenesulfonamide

CHEMICAL NAME

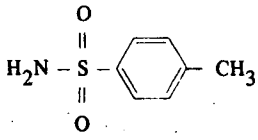
CAS Number: 70-55-3

Chemical Name: p-Toluene sulfonylamide

Synonyms: ρ-Toluene sulfonamide
4-Toluenesulfonic acid, amide

Molecular Formula: $C_7H_9NO_2S$

Structure:



Chemical Properties

Molecular Weight: 171.22

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point: 138.5 to 139°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
LD_{50}	75 mg/kg	wild bird	oral
	250 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

o-Toluenesulfonic acid

CHEMICAL NAME

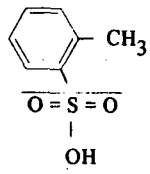
CAS Number: 88-20-0

Chemical Name: o-Toluenesulfonic acid

Synonyms: o-Toluenesulfonate
2-Toluenesulfonic acid

Molecular Formula: $C_7H_8O_3S$

Structure:



Chemical Properties

Molecular Weight: 172.21

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 128.8°C at 25 mm

Melting Point: 67.5°C

Density:

Solubility: Very 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**

Non-lethal Acute Effects:

High irritant
Moderate systemic toxicity

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

p-Toluenesulfonic acid

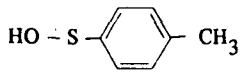
CHEMICAL NAME

CAS Number: 104-15-4

Chemical Name: p-Toluenesulfonic acid

Synonyms: p-Toluene sulfonate

Molecular Formula: $C_7H_8O_3S$

Structure: 

Chemical Properties

Molecular Weight: 172.21

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 140°C at 20 mm

Melting Point: 104 to 105°C

Density:

Solubility: Very soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

p-Toluenesulfonic 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
LD_{50}	400 mg/kg	rat	oral

Non-lethal Acute Effects:

High irritant
Moderate systemic toxicity

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Toluenesulfonyl chloride

CHEMICAL NAME

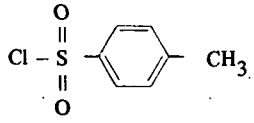
CAS Number: 98-59-9

Chemical Name: p-Toluenesulfonyl chloride

Synonyms:

Molecular Formula: $C_7H_7ClO_2S$

Structure:



Chemical Properties

Molecular Weight: 190.65

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 145 to 146°C at 15 mm

Melting Point: 71°C

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

Non-lethal Acute Effects:

Severe irritant

Moderate systemic toxicity

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

m-Toluidine

CHEMICAL NAME

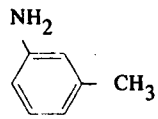
CAS Number: 108-44-1

Chemical Name: m-Toluidine

Synonyms: m-Methyl aniline
3-Aminotoluene
3-Amino-1-methylbenzene

Molecular Formula: C_7H_9N

Structure:



Chemical Properties

Molecular Weight: 107.16

Physical State: Liquid

Vapor Pressure: 1 mm at 41°C

Vapor Density: 3.90

Boiling Point: 200.23°C at 760 mm

Melting Point: -14.7°C

Density: 0.9984 at 20°C/4°C

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient: 1.60

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
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}	974 mg/kg	rat	oral
	150 mg/kg	mouse	intraperitoneal

Non-lethal Acute Effects:

Local irritant
Allergies
Headache
Irritation
Difficulty in breathing
Psychic disturbances
Marked irritation of the kidneys and bladder

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplasm:

TD_{Lo}	6600 μg/kg (19 weeks)	rat	oral

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

o-Toluidine

CHEMICAL NAME

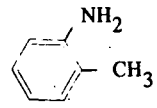
CAS Number: 95-53-4

Chemical Name: o-Toluidine

Synonyms: o-Methyl aniline
2-Methyl aniline
2-Amino toluene

Molecular Formula: C_7H_9N

Structure:



Chemical Properties

Molecular Weight: 107.16

Physical State: Liquid

Vapor Pressure: 1 mm at 44°C

Vapor Density: 3.69

Boiling Point: 200.23°C at 760 mm

Melting Point: -23.7°C (unstable)
-14.7°C (stable)

Density: 0.9984 at 20°C/4°C

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient: 1.61

Environmental Persistence

BOD: 45% of theoretical

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}	900 mg/kg	rat	oral
	150 mg/kg	mouse	intraperitoneal
	3250 mg/kg	rabbit	skin
LD_{Lo}	300 mg/kg	cat	oral
	5 mg/kg	frog	oral

Non-lethal Acute Effects:

Difficulty in breathing
Headache
Marked irritation of kidneys and bladder
Psychic disturbance

Chronic Toxicity

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

Carcinogenicity:

Neoplasm TD_{Lo}	8200 mg/kg (24 weeks)	rat	oral

Mutagenicity:

Teratogenicity:

TLV: 5 ppm (skin)

Other Chronic Effects:

p-Toluidine

CHEMICAL NAME

CAS Number: 106-49-0

Chemical Name: p-Toluidine

Synonyms: p-Methyl aniline
4-Amino toluene

Molecular Formula: C_7H_9N

Structure: 

Chemical Properties

Molecular Weight: 107.16

Physical State: Solid

Vapor Pressure: 1 mm at 42°C

Vapor Density: 3.90

Boiling Point: 200.55°C at 760 mm

Melting Point: 43.7°C

Density: 0.9619 at 20°C/4°C

Solubility: Slightly (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}	50 mg/kg	mouse	intraperitoneal
	42 mg/kg	wild bird	oral
LD_{Lo}	100 mg/kg	mammal	oral

Non-lethal Acute Effects:

Difficulty in breathing
Kidney damage

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Recognized carcinogen

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Toxaphene

CHEMICAL NAME

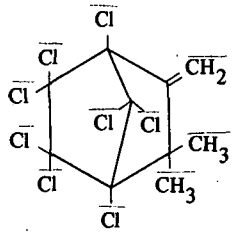
CAS Number: 8001-35-2

Chemical Name: Toxaphene

Synonyms: Chlorinated camphene
Strobane
Alltox
Geniphene

Molecular Formula: $C_{10}H_8Cl_8$

Structure:



Chemical Properties

Molecular Weight: 413.84

Physical State: Solid

Vapor Pressure: 0.2 to 0.4 mm at 25°C

Vapor Density:

Boiling Point: Decomposes

Melting Point: 65 to 90°C

Density: 1.66 at 20°C

Solubility: 3 ppm at 25°C (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

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

Toxaphene

PRODUCTION DATA

Annual U.S. Production: 48 x 10^6 lbs.

Consumption: 48 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 50.5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	60 mg/kg	rat	oral
	780 mg/kg	rat	skin
	1025 mg/kg	rabbit	skin
	71 mg/kg	duck	oral
LD_{Lo}	40 mg/kg	human	oral
	2000 mg/m^3 (2 hours)	mouse	inhalation
	180 mg/kg	mouse	interperitoneal
	50 mg/kg	dog	oral
	780 mg/kg	rabbit	oral

Non-lethal Acute Effects:

Nausea and vomiting
Muscle cramps
Irritation of respiratory tract

Chronic Toxicity

U.S. Occupational Standard: 7 ppm for food residues

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 500 $\mu g/m^3$

Other Chronic Effects:

Tributyl phosphate

CHEMICAL NAME

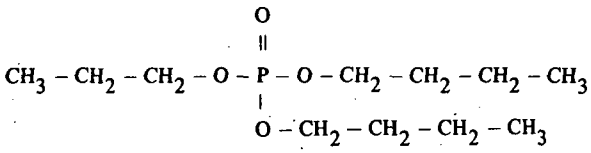
CAS Number: 126-73-8

Chemical Name: Phosphoric acid, tributyl ester

Synonyms: Tributyl phosphate

Molecular Formula: $C_{12}H_{27}O_4P$

Structure:



Chemical Properties

Molecular Weight: 266.32

Physical State: Liquid

Vapor Pressure: 20 mm at 20°C

Vapor Density: 9.20

Boiling Point: 289°C

Melting Point:

Density: 0.9727 at 25°C/4°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Disaster hazard–dangerous phosphates

Tributyl phosphate

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
LD_{Lo}	63 mg/kg	mouse	intraperitoneal

Non-lethal Acute Effects:
Stimulation of CNS

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 5 ppm

Other Chronic Effects:

Trichloroaniline

CHEMICAL NAME

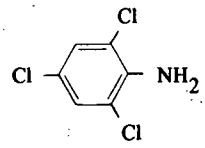
CAS Number: 634-93-5

Chemical Name: 2,4,6-Trichloroaniline

Synonyms: Trichloroaniline
sym-Trichloroaniline

Molecular Formula: $C_6H_4Cl_3N$

Structure:



Chemical Properties

Molecular Weight: 196.46

Physical State: Solid

Vapor Pressure: 1 mm at 134°C

Vapor Density:

Boiling Point: 262°C at 746 mm

Melting Point: 78.5°C

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

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Trichlorobenzene

CHEMICAL NAME

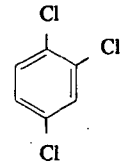
CAS Number: 120-82-1

Chemical Name: 1,2,4-Trichlorobenzene

Synonyms:

Molecular Formula: $C_6H_3Cl_3$

Structure:



Chemical Properties

Molecular Weight: 181.45

Physical State: Liquid

Vapor Pressure: 1 mm at 40°C

Vapor Density: 6.26

Boiling Point: 213.5°C at 760 mm

Melting Point: 16.95°C

Density: 1.4542 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–chlorides

PRODUCTION DATA

Annual U.S. Production: 10×10^6 lbs. (1975 estimate)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	756 mg/kg	rat	oral
	766 mg/kg	mouse	oral
LD_{Lo}	500 mg/kg	mouse	intraperitoneal

Non-lethal Acute Effects:
Local irritant
Causes loss of hair

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

1, 1, 1-Trichloroethane

CHEMICAL NAME

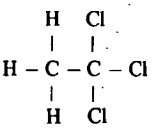
CAS Number: 71-55-6

Chemical Name: 1,1,1-Trichloroethane

Synonyms: α-Trichloroethane
Methyl chloroform

Molecular Formula: $C_2H_3Cl_3$

Structure:



Chemical Properties

Molecular Weight: 133.41

Vapor Pressure: 130.86 at 25°C

Boiling Point: 74.1°C at 760 mm

Density: 1.3390 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 4.55

Melting Point: -30.41°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–chlorides

1, 1, 1-Trichloroethane

PRODUCTION DATA

Annual U.S. Production: 591 x 10^6 lbs. (1974)

Consumption: 591 x 10^6 lbs.

Fraction of Dispersion: 0.73

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 284.5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	5660 mg/kg	rabbit	oral
	9470 mg/kg	guinea pig	oral

Non-lethal Acute Effects:

Psychotrophic effects:

TC_{Lo}	350 ppm	human male	inhalation

CNS effects:

TC_{Lo}	920 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 350 ppm

Other Chronic Effects:

Reduced growth
Reversible dystrophic changes in liver, kidneys, myocardium and lungs
Narcotic effect

1, 1, 2-Trichloroethane

CHEMICAL NAME

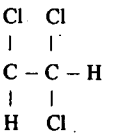
CAS Number: 79-00-5

Chemical Name: 1,1,2-Trichloroethane

Synonyms: Vinyl trichloride
β-Trichloroethane

Molecular Formula: $C_2H_3Cl_3$

Structure:



Chemical Properties

Molecular Weight: 133.41

Physical State: Liquid

Vapor Pressure: 25 mm at 25°C

Vapor Density:

Boiling Point: 113.77°C at 760 mm

Melting Point: -36.5°C

Density: 1.4397 at 20°C/4°C

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

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

1, 1, 2-Trichloroethane

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
	227 mg/kg	mouse	subcutaneous
LD_{Lo}	750 mg/kg	dog	oral
	95 mg/kg	dog	intravenous
	500 mg/kg	rabbit	subcutaneous
LC_{Lo}	500 ppm (8 hours)	rat	inhalation

Non-lethal Acute Effects:

Psychotic effects:

TC_{Lo}	350 ppm	man	inhalation
CNS effects	920 ppm	human	inhalation

Chronic Toxicity

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

Carcinogenicity:

Not carcinogenic according to Dow Chemical Co. after 12-month test

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Trichloroethylene

CHEMICAL NAME

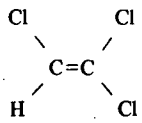
CAS Number: 79-01-6

Chemical Name: Trichloroethylene

Synonyms: Ethylene trichloride
Trichloroethene
Ethinyl trichloride
Acetylene trichloride

Molecular Formula: C_2HCl_3

Structure:



Chemical Properties

Molecular Weight: 131.39

Physical State: Liquid

Vapor Pressure: 77.5 mm at 25°C

Vapor Density: 4.53

Boiling Point: 87°C at 760 mm

Melting Point: -73°C

Density: 1.4642 at 20°C/4°C

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Common air contaminant
Slowly oxidized by O_3 and RO_2; products are phosgene, HCl, CO, trichloroethylene oxide and dichloroacetylchloride
Unreactive towards OH

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

Trichloroethylene

PRODUCTION DATA

Annual U.S. Production: 285.2 x 10^6 lbs. (1975)

Consumption: 370 to 390 x 10^6 lbs. (1975 estimate)

Fraction of Dispersion: 0.95

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 429.5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	4920 mg/kg	rat	oral
	34 mg/kg	mouse	intravenous
	1900 mg/kg	dog	intraperitoneal
LD_{Lo}	857 mg/kg	human	oral
	1800 mg/kg	rabbit	subcutaneous
	5860 mg/kg	dog	oral
	150 mg/kg	dog	intravenous
LC_{Lo}	3000 ppm (2 hours)	mouse	inhalation
	11,000 ppm	rabbit	inhalation
	8000 ppm (8 hours)	rat	inhalation

Non-lethal Acute Effects:

CNS effects

TC_{Lo}	160 ppm (83 minutes)	human	inhalation

Conjunctivitis

Irritation of skin and respiratory tract

Chronic Toxicity

U.S. Occupational Standard: (air)

TWA	100 ppm
Ceiling	200 ppm (recommended 150 ppm)
Peak	300 ppm/5 minutes/2 hours

Carcinogenicity:

TD_{Lo}	351 gm/kg (78 weeks)	mouse	oral

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Kidney, spleen, and liver damage
Metabolic and enzymatic effects
Hypertension
Decreased ATP level
Reduces antibody formation

Trichlorofluoromethane

CHEMICAL NAME

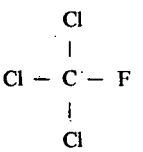
CAS Number: 75-69-4

Chemical Name: Trichlorofluoromethane

Synonyms: Freon 11
Monofluorotrichloromethane

Molecular Formula: CCl_3F

Structure:



Chemical Properties

Molecular Weight: 137.38

Physical State: Liquid

Vapor Pressure: 717.5 mm at 25°C

Vapor Density:

Boiling Point: 24.1°C

Melting Point:

Density: 1.494 at 17.2°C

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–toxic fumes–chlorides and fluorides

Trichlorofluoromethane

PRODUCTION DATA

Annual U.S. Production: 299.6 x 10^6 lbs.

Consumption: 299.6 x 10^6 lbs.

Fraction of Dispersion: 0.90

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 274.1

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Non-lethal Effects:
Narcosis
Anesthesia
Cardiotoxic

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 1000 ppm

Other Chronic Effects:

Trichloroisocyanuric acid

CHEMICAL NAME

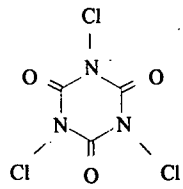
CAS Number: 87-90-1

Chemical Name: 1,3,5-Trichloro-s-triazine-2,4,6(1H,3H,5H)-trione

Synonyms: Trichloroisocyanuric acid
Trichlorotriozinetrione

Molecular Formula: $C_3Cl_3N_3O_3$

Structure:



Chemical Properties

Molecular Weight: 232.5

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point: 225 to 230°C

Density:

Solubility: Soluble (12 gm/l H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous Cl and CO gases

Trichloroisocyanuric acid

PRODUCTION DATA

Annual U.S. Production: 40×10^6 lbs.

Consumption: 40×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 41.2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	750 mg/kg	rat	oral

Non-lethal Acute Effects:
Irritant to skin and tissue

Chronic Toxicity

U.S. Occupational Standard:
FDA regulation for use as sanitizing agent:
100 ppm Cl^- in aqueous solution

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Trichloronaphthalene

CHEMICAL NAME

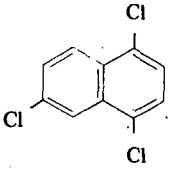
CAS Number: 2437-54-9

Chemical Name: 1,4,6-Trichloronaphthalene

Synonyms:

Molecular Formula: $C_{10}H_5Cl_3$

Structure:



Chemical Properties

Molecular Weight:	231.51	Physical State:	Solid
Vapor Pressure:		Vapor Density:	
Boiling Point:		Melting Point:	
Density:		Solubility:	
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–chlorides

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:			
Systemic effects:			
TC_{Lo}	30 mg/kg	human	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Trichlorophenoxyacetic acid

CHEMICAL NAME

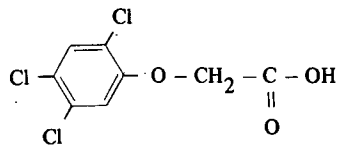
CAS Number: 93-76-5

Chemical Name: (2,4,5-Trichlorophenoxy)acetic acid

Synonyms: 2,4,5-Trichlorophenoxyacetic acid
2,4,5-T

Molecular Formula: $C_8H_5Cl_3O_3$

Structure:



Chemical Properties

Molecular Weight: 255.49

Physical State: Solid

Vapor Pressure: Low

Vapor Density:

Boiling Point:

Melting Point: 157 to 158°C

Density: 1.80 at 20°C/20°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard—dangerous chlorides

Trichlorophenoxyacetic acid

PRODUCTION DATA

Annual U.S. Production: 6.0×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 6.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	500 mg/kg	male rat	oral
	300 mg/kg	rat	oral
	500 mg/kg	rat	unreported
	389 mg/kg	mouse	oral
	100 mg/kg	dog	oral
	381 mg/kg	guinea pig	oral
	310 mg/kg	chicken	oral
	500 mg/kg	mammal	oral

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TD_{Lo}	100 mg/kg	rat (6-15 days–pregnant)	oral
	<150 μg/kg	mouse (6-14 days–pregnant)	subcutaneous

(The teratogenicity is due in part to 2,3,7,8-TCDD (2,3,7,8-tetrachlorodibenzo-p-dioxin) which is present as a contaminant)

Other Chronic Effects:

TLV:

Trichloropropane

CHEMICAL NAME

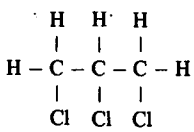
CAS Number: 96-18-4

Chemical Name: 1,2,3-Trichloropropane

Synonyms: Glycerol trichlorohydrin
Allyl trichloride trichlorohydrin

Molecular Formula: $C_3H_5Cl_3$

Structure:



Chemical Properties

Molecular Weight: 147.43

Physical State: Liquid

Vapor Pressure: 3.59 mm at 25°C

Vapor Density: 5.0

Boiling Point: 156.85°C at 760 mm

Melting Point: -14.7°C

Density: 1.3889 at 20°C/4°C

Solubility: Slightly (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

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}	320 mg/kg	rat	oral
	1770 mg/kg	rabbit	skin
LD_{Lo}	200 mg/kg	dog	oral
LC_{Lo}	1000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Local irritant
Lesions in liver, kidney and heart

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 50 ppm

Other Chronic Effects:

Trichlorotrifluoroethane

CHEMICAL NAME

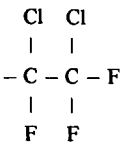
CAS Number: 76-13-1

Chemical Name: 1,1,2-Trichloro-1,2,2-trifluoroethane

Synonyms: Trifluorotrichloroethane

Molecular Formula: $C_2Cl_3F_3$

Structure:



Chemical Properties

Molecular Weight: 187.38

Physical State: Liquid

Vapor Pressure: 337.72 mm at 25°C

Vapor Density: 6.47

Boiling Point: 47.7°C at 760 mm

Melting Point: -36.4°C

Density: 1.5635 at 25°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Stable in lower atmosphere

Safety Hazard:
Fire–slight
Disaster hazard–dangerous–toxic fumes–fluorides and chlorides

Trichlorotrifluoroethane

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr): 682 (1973 emissions of F-11 and F-12)

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

TC_{Lo}	4500 ppm	human	inhalation

Mutagenicity:

Teratogenicity:

TLV: 1000 ppm

Other Chronic Effects:

Tricresyl phosphate

CHEMICAL NAME

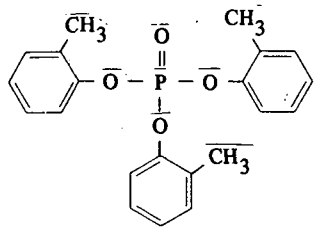
CAS Number: 78-30-8

Chemical Name: Phosphoric acid, tri-o-tolyl ester

Synonyms: o-Tolyl phosphate
Tricresyl phosphate
Tri-o-cresyl phosphate
Tri-o-tolyl phosphate
Tri-2-tolyl phosphate

Molecular Formula: $C_{21}H_{21}O_4P$

Structure:



Chemical Properties

Molecular Weight: 368.37

Physical State: Liquid

Vapor Pressure: 0.29 mm at 200°C

Vapor Density: 12.7

Boiling Point: 410°C

Melting Point: 11°C

Density: 1.1955 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 PO_x

Tricresyl phosphate

PRODUCTION DATA

Annual U.S. Production: 50.2×10^6 lbs.

Consumption: 42.7×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 43.5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	4680 mg/kg	rat	oral
	500 mg/kg	dog	oral
	100 mg/kg	rabbit	oral

Non-lethal Acute Effects:

CNS effects, paralysis
Nausea and vomiting

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 0.1 mg/m^3

Carcinogenicity: Negative result in 12-week rat study

Mutagenicity:

Teratogenicity:

TLV: 0.1 mg/m^3

Other Chronic Effects:

Tridecylbenzenesulfonic acid, sodium salt

CHEMICAL NAME

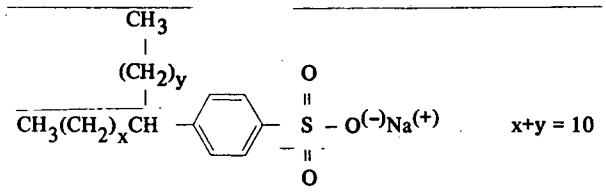
CAS Number: 14356-40-2

Chemical Name: p-Tridecylbenzenesulfonic acid, sodium salt

Synonyms:

Molecular Formula: $C_{19}H_{32}O_3S \cdot Na$

Structure:



x+y = 10

Chemical Properties

Molecular Weight: 361.50

Physical State:

Vapor Pressure: Negligible at 25°C

Vapor Density:

Boiling Point:

Melting Point:

Density:

Solubility:

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Tridecylbenzenesulfonic acid, sodium salt

PRODUCTION DATA

Annual U.S. Production: 149.9 x 10^6 lbs.

Consumption: 149.9 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 152.1

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Triethanolamine

CHEMICAL NAME

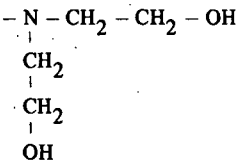
CAS Number: 102-71-6

Chemical Name: 2,2',2",-Nitrilotriethanol

Synonyms: Triethanolamine
2,2',2"-Trihydroxyethylamine

Molecular Formula: $C_6H_{15}NO_3$

Structure:



Chemical Properties

Molecular Weight:	149.19	**Physical State:**	Solid–liquid
Vapor Pressure:	<0.01 mm at 20°C	**Vapor Density:**	5.14
Boiling Point:	277°C at 150 mm	**Melting Point:**	21.2°C
Density:	1.1242 at 20°C/4°C	**Solubility:**	Infinite (H_2O)
Octanol/Water Partition Coefficient:	-1.75		

Environmental Persistence

BOD: 66% of theoretical after 10 days at 20°C at 10 mg/l
Total theoretical oxygen demand = 2.04 gm/gm
Resistance to biodegradation

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–slight
Disaster hazard–dangerous–NO_x

Triethanolamine

PRODUCTION DATA

Annual U.S. Production: 100.7 x 10^6 lbs.

Consumption: 85.7 x 10^6 lbs.

Fraction of Dispersion: 0.40

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 35.8

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	8000 mg/kg	guinea pig	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Triethylamine

CHEMICAL NAME

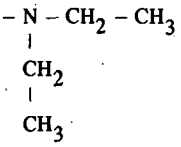
CAS Number: 121-44-8

Chemical Name: Triethylamine

Synonyms: N,N-Diethylethanamine

Molecular Formula: $C_6H_{15}N$

Structure:



Chemical Properties

Molecular Weight: 101.19

Physical State: Liquid

Vapor Pressure:

Vapor Density: 3.48

Boiling Point: 89.3°C at 760 mm

Melting Point: -114.7°C

Density: 0.7275 at 20°C/4°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient: 1.37

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:

Fire–dangerous

Triethylamine

PRODUCTION DATA

Annual U.S. Production: 22.8×10^6 lbs. (1967) (Includes monoethylamine)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	460 mg/kg	rat	oral
	546 mg/kg	mouse	oral
	570 mg/kg	rabbit	skin
LC_{Lo}	1000 ppm (4 hours)	rat	inhalation
	1000 ppm (4 hours)	guinea pig	inhalation

Non-lethal Acute Effects:

Liver and kidney damage
Irritant to skin and mucous membranes

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 25 ppm

Other Chronic Effects:

Triethylene glycol

CHEMICAL NAME

CAS Number: 112-27-6

Chemical Name: Triethylene glycol

Synonyms: 2,2'-Ethylene dioxy diethanol glycol
Bis (hydroxyethyl) ether

Molecular Formula: $C_6H_{14}O_4$

Structure:

$$CH_2 - O - CH_2 - CH_2 - OH$$
$$|$$
$$CH_2 - O - CH_2 - CH_2 - OH$$

Chemical Properties

Molecular Weight: 150.18

Physical State: Liquid

Vapor Pressure: 1 mm at 114°C

Vapor Density:

Boiling Point: 278.3°C at 760 mm

Melting Point: -5°C

Density: 1.1274 at 15°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient: -2.08

Environmental Persistence

BOD: 85% of theoretical after 20 days at 20°C
Total theoretical oxygen demand = 1.6 gm/gm

Atmospheric Reactivity:

Safety Hazard:
Fire–slight
Explosion–moderate

Triethylene glycol

PRODUCTION DATA

Annual U.S. Production: 113 x 10^6 lbs.

Consumption: 113 x 10^6 lbs.

Fraction of Dispersion: 0.75

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 70.8

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	9739 mg/kg	mouse	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Triethylene glycol, dimethyl ether

CHEMICAL NAME

CAS Number: 112-49-2

Chemical Name: 2,5,8,11-Tetraoxadodecane

Synonyms: Triethyleneglycol dimethyl ether
Triglyme
1,2-Bis(2-methoxyethoxy)ethane

Molecular Formula: $C_8H_{18}O_4$

Structure: $CH_3 - (OCH_2CH_2)_3 - OCH_3$

Chemical Properties

Molecular Weight: 178.22

Physical State: Liquid

Vapor Pressure: 0.9 mm at 20°C

Vapor Density:

Boiling Point: 216°C

Melting Point: –46°C

Density: 0.9862 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–slight

Triethylene 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 (Low toxicity)	**Dosage**	**Animal**	**Route**

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Triethylene glycol, monomethyl ether

CHEMICAL NAME

CAS Number: 112-35-6

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

Synonyms: Triethylene glycol, monomethyl ether
Methoxytriglycol
Methoxytriethylene glycol

Molecular Formula: $C_7H_{16}O_4$

Structure: $CH_3 - (OCH_2CH_2)_3 - OH$

Chemical Properties

Molecular Weight: 164.20

Physical State:

Vapor Pressure: <0.01 mm at 20°C

Vapor Density:

Boiling Point: 249°C

Melting Point:

Density: 1.0494

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–slight

Triethylene glycol, monomethyl ether

PRODUCTION DATA

Annual U.S. Production: 31.7×10^6 lbs.

Consumption: 26.7×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 27.2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Trifluralin

CHEMICAL NAME

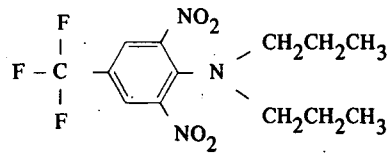
CAS Number: 1582-09-8

Chemical Name: α,α,α,-Trifluoro-2, 6-dinitro-N, N-dipropyl-p-toluidine

Synonyms: Trifluralin

Molecular Formula: $C_{13}H_{16}F_3N_3O_4$

Structure:



Chemical Properties

Molecular Weight: 335.32

Physical State: Solid

Vapor Pressure: 1.99×10^{-4} mm at 29.5°C

Vapor Density:

Boiling Point: 139 to 140°C at 4.2 mm

Melting Point: 48.5 to 49°C

Density:

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Degraded by ultraviolet irradiation

Safety Hazard:
Disaster hazard—dangerous nitrates and fluorides

PRODUCTION DATA

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

Consumption: 20 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 20.2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	>10,000 mg/kg	rat	oral
	5 gm/kg	mouse	oral
	5000 gm/kg	mouse	oral
	500 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Triisobutylene

CHEMICAL NAME

CAS Number: 9003-27-4

Chemical Name: 2-Methyl-1-propene, homopolymer

Synonyms: Triisobutylene
2-Methylpropene (trimer)
Poly(2-methylpropene)
Polyisobutylene

Molecular Formula: $C_{12}H_{24}$

Structure: (mixture of isomers)

Chemical Properties

Molecular Weight: 168.33

Physical State: Liquid

Vapor Pressure: 2.08 mm at 25°C

Vapor Density:

Boiling Point: 179 to 181°C

Melting Point: -76°C

Density: 0.7590 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Triisobutylene

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:

Trimethylamine

CHEMICAL NAME

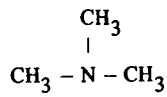
CAS Number: 75-50-3

Chemical Name: Trimethylamine

Synonyms: N,N-Dimethylmethanamine

Molecular Formula: C_3H_9N

Structure:



Chemical Properties

Molecular Weight: 59.11

Physical State: Gas

Vapor Pressure: 687 mm at 0°C

Vapor Density: 2.0

Boiling Point: 2.87°C at 760 mm

Melting Point: -117.2°C

Density: 0.6356 at 20°C/4°C

Solubility: Very (H_2O)

Octanol/Water Partition Coefficient: 1.45

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:

Fire–moderate
Explosion–moderate
Disaster hazard–moderate–toxic fumes

Trimethylamine

PRODUCTION DATA

Annual U.S. Production: 28.8×10^6 lbs.

Consumption: 28.8×10^6 lbs.

Fraction of Dispersion: 0.70

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 20.6

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	90 mg/kg	mouse	intravenous
LD_{Lo}	75 mg/kg	mouse	intraperitoneal
	1000 mg/kg	mouse	subcutaneous
	800 mg/kg	rabbit	subcutaneous
	400 mg/kg	rabbit	intravenous
	2000 mg/kg	frog	subcutaneous

Non-lethal Acute Effects:
Irritant to skin, respiratory organs

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Trimethylpentanediol

CHEMICAL NAME

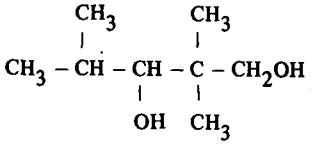
CAS Number: 144-19-4

Chemical Name: 2,2,4-Trimethyl-1,3-pentanediol

Synonyms: TMPD

Molecular Formula: $C_8H_{18}O_2$

Structure:



Chemical Properties

Molecular Weight: 146.23

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 234°C at 737 mm

Melting Point: 51.8 to 52.2°C

Density: 0.937 at 15°C/15°C

Solubility: Slightly (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: 20 x 10^6 lbs.

Consumption: 20 x 10^6 lbs.

Fraction of Dispersion: 0.8

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 16.3

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Trinitrotoluene

CHEMICAL NAME

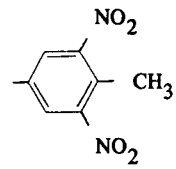
CAS Number: 118-96-7

Chemical Name: 2,4,6-Trinitrotoluene

Synonyms: Trinitrotoluene
TNT
sym-Trinitrotoluene
Triton
s-Trinitrotoluene

Molecular Formula: $C_7H_5N_3O_6$

Structure:



Chemical Properties

Molecular Weight: 227.13

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 290 to 310°C (explodes)

Melting Point: 104°C

Density: 1.654

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Explosion–moderate
Disaster hazard–highly 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
TD_{Lo}	700 mg/kg	rat	oral
	1850 mg/kg	cat	oral
	200 mg/kg	cat	subcutaneous
	500 mg/kg	rabbit	oral
	500 mg/kg	rabbit	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Trithion

CHEMICAL NAME

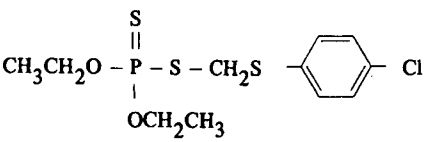
CAS Number: 786-19-6

Chemical Name: Phosphorodithioic acid, S-[[(p-Chlorophenyl)thio]methyl]O, O-diethyl ester

Synonyms: Trithion
O,O-diethyl-S-p-chlorophenylthiomethyl phosphorodithioate
Carbophenothion

Molecular Formula: $C_{11}H_{16}ClO_2PS_3$

Structure:



Chemical Properties

Molecular Weight: 260.39

Vapor Pressure: Negligible

Boiling Point: 82°at 0.01 mm

Density: 1.280 to 1.285 at 20°C/20°C

Octanol/Water Partition Coefficient:

Physical State:

Vapor Density:

Melting Point:

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous phosphates and chlorides

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}	32 mg/kg	male rat	oral
	10 mg/kg	rat	oral
	27 mg/kg	rat	skin
	11 mg/kg	rat	intraperitoneal
	218 mg/kg	mouse	oral
	27 mg/kg	mouse	intraperitoneal
	1270 mg/kg	rabbit	skin
	57 mg/kg	chicken	oral
	6 mg/kg	wild bird	oral

Non-lethal Acute Effects:
Pulmonary edema
Convulsions

Chronic Toxicity

U.S. Occupational Standard: EPA farm worker reentry standard

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Urea

CHEMICAL NAME

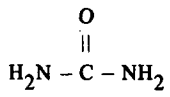
CAS Number: 57-13-6

Chemical Name: Urea

Synonyms: Carbamide
Carbonyldiamine

Molecular Formula: CH_4N_2O

Structure:



Chemical Properties

Molecular Weight: 60.06

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: (Decomposes)

Melting Point: 135°C

Density: 1.3230 at 20°C/4°C

Solubility: Very soluble (H_2O)

Octanol/Water Partition Coefficient: −2.96

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 8,390 x 10^6 lbs. (1975)

Consumption: 8,420 x 10^6 lb.s (1975)

Fraction of Dispersion:

Fraction of Production Lost: 0.15

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	3000 mg/kg	dog	subcutaneous
	3000 mg/kg	dog	intravenous
	3000 mg/kg	rabbit	subcutaneous
	600 mg/kg	frog	subcutaneous
	511 mg/kg	domestic	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Vernam

CHEMICAL NAME

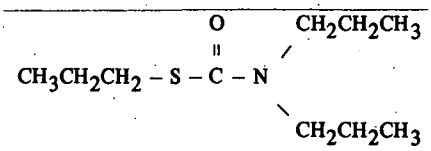
CAS Number: 1929-77-7

Chemical Name: Dipropylcarbamothioic acid, S-propyl ester

Synonyms: S-Propyldipropylthiocarbamate

Molecular Formula: $C_{10}H_{21}NOS$

Structure:



Chemical Properties

Molecular Weight: 203.38

Physical State: Liquid

Vapor Pressure: 10.4×10^{-3} mm at 25°C

Vapor Density:

Boiling Point: 150°C at 30 mm

Melting Point:

Density: 0.95 at 20°C/20°C

Solubility: 90 ppm 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: Estimated as 1.0

Fraction of Production Lost:

Release Rate (million lbs/yr): 2.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1800 mg/kg	rat	oral
	1470 mg/kg	rat	oral
	1780 mg/kg	rat	unreported

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Vinyl acetate

CHEMICAL NAME

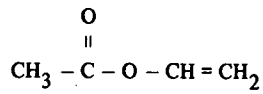
CAS Number: 108-05-4

Chemical Name: Vinyl acetate

Synonyms: Acetic acid, vinyl ester
Acetic acid, ethenyl ester

Molecular Formula: $C_4H_6O_2$

Structure:



Chemical Properties

Molecular Weight: 86.09

Physical State: Liquid (polymerizes)

Vapor Pressure: 107.5 mm at 25°C

Vapor Density: 3.0

Boiling Point: 72.2 to 72.3°C at 760 mm

Melting Point: -93.2°C

Density: 0.9317 at 20°C/4°C

Solubility: Insoluble (H_2O)
Soluble in hot H_2O

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 72% of theoretical after 20 days at 20°C
Total theoretical oxygen demand = 1.67 gm/gm

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–highly dangerous

PRODUCTION DATA

Annual U.S. Production: 1210.7 x 10^6 lbs.

Consumption: 989.4 x 10^6 lbs.

Fraction of Dispersion: 0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 18.2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2920 mg/kg	rat	oral
	2320 mg/kg	rabbit	skin
LD_{Lo}	500 mg/kg	rat	intraperitoneal
LC_{Lo}	4000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Skin irritant

Vapors may be narcotic

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

Other Chronic Effects:

TLV: TWA 10 ppm

Odor perception: 0.12 ppm

Vinyl chloride

CHEMICAL NAME

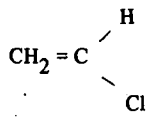
CAS Number: 75-01-4

Chemical Name: Chloroethylene

Synonyms: Vinyl chloride
Chloroethene

Molecular Formula: C_2H_3Cl

Structure:



Chemical Properties

Molecular Weight: 62.50

Physical State: Liquid or gas

Vapor Pressure: 2660 mm at 25°C

Vapor Density: 2.15

Boiling Point: -13.4°C at 760 mm

Melting Point: −153.8°C

Density: 0.9195 at 15°C/4°C

Solubility: Slightly (1.1 gm/l H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: Total theoretical oxygen demand = 1.28 gm/gm

Atmospheric Reactivity: Reacts with oxidizing materials
Activity toward O_3: $t_{1/2}$ = <3 days
RO_2: $t_{1/2} = 10^3$ days; slow oxidation in water
OH: $t_{1/2}$ = 3 days

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

PRODUCTION DATA

Annual U.S. Production: 5088.5 x 10^6 lbs. (4,174.6 x 10^6 lbs., 1975)

Consumption: 4467.6 x 10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.02

Release Rate (million lbs/yr): 146.5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LC	100,000 to 400,000 ppm	mouse	unknown
		dog	unknown
		cat	unknown
		guinea pig	unknown

Non-lethal Acute Effects:

Cardiovascular			
TC_{Lo}	20 ppm	human	inhalation
Paralysis			
TC_{Lo}	300 ppm	human	inhalation
Skin irritation			
Conjunctivitis			

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 1 ppm; Ceiling 5 ppm

Carcinogenicity:

LC_{Lo}	250 ppm (4 hours/ 260 days)	rat	inhalation

Mutagenicity:
Positive: Ames *Salmonella*

Teratogenicity:

TLV: 500 ppm or 1300 mg/m^3

Other Chronic Effects:
Liver and kidney damage
Cardiovascular damage
Thyroid and brain degeneration

Vinylidene chloride

CHEMICAL NAME

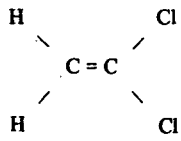
CAS Number: 75-35-4

Chemical Name: 1,1-Dichloroethylene

Synonyms: Vinylidene chloride

Molecular Formula: $C_2H_2Cl_2$

Structure:



Chemical Properties

Molecular Weight: 97.0

Physical State: Volatile liquid

Vapor Pressure: 617.14 mm at 25°C

Vapor Density:

Boiling Point: 37°C at 760 mm

Melting Point: -122.53°C

Density: 1.213 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials
Activity towards O_3: $t_{1/2}$ <1 day
RO_2: $t_{1/2} = 10^3$ days
OH: $t_{1/2}$ <1 day, producing phosgene and formaldehyde

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

Vinylidene chloride

PRODUCTION DATA

Annual U.S. Production: 260 x 10^6 lbs.

Consumption: 54 x 10^6 lbs.

Fraction of Dispersion: 0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 2.4

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	3700 mg/kg	rabbit	subcutaneous
	5750 mg/kg	dog	oral
	225 mg/kg	dog	intravenous
LC_{Lo}	10,000 ppm	rat	inhalation

Non-lethal Acute Effects:

Irritant to eyes, skin, and respiratory tract
Narcosis

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Suspected

Mutagenicity: Positive: Ames bacterial system

Teratogenicity:

TLV: 25 ppm (suggested)
Odor perception: 1000 ppm

Other Chronic Effects:

Vinyltoluene

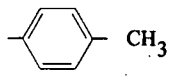
CHEMICAL NAME

CAS Number: 622-97-9

Chemical Name: p-Methylstyrene

Synonyms: Vinyltoluene

Molecular Formula: C_9H_{10}

Structure: 

Chemical Properties

Molecular Weight: 118.2

Physical State: Liquid

Vapor Pressure: 1.15 mm at 20°C

Vapor Density: 4.08

Boiling Point: 170 to 171°C

Melting Point:

Density: Monomer: 0.89 at 25°C/25°C
Polymer: 1.027 at 25°C/25°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing material forming formaldehyde and methylbenzaldehyde
Activity toward RO_2: $t_{1/2}$ = 24 hours
O_3: $t_{1/2}$ = 24 hours
OH: $t_{1/2}$ = 1 day

Safety Hazard:
Fire–moderate

PRODUCTION DATA

Annual U.S. Production: 40×10^6 lbs.

Consumption: 40×10^6 lbs.

Fraction of Dispersion: 0.30

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 12.6

TOXICITY DATA

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

Non-lethal Acute Effects:

Irritation

$\overline{TC}_{Lo}$	400 ppm	human	inhalation

Damaged kidneys and liver

Irritant to eye, nose and throat

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 1000 ppm

Other Chronic Effects:

Warfarin

CHEMICAL NAME

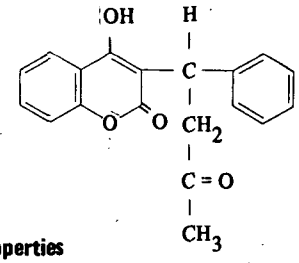
CAS Number: 81-81-2

Chemical Name: 3-(α-Acetonylbenzyl)-4-hydroxycoumarin)

Synonyms: Warfarin
WARF-42
Compound 42

Molecular Formula: $C_{19}H_{16}O_4$

Structure:



Chemical Properties

Molecular Weight:	308.35	Physical State:	Solid
Vapor Pressure:		Vapor Density:	
Boiling Point:		Melting Point:	161°C
Density:		Solubility:	Insoluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 12.0 x 10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 13.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	58 to 323 mg/kg	rat	oral
	3 mg/kg	rat	oral
	186 mg/kg	rat	intravenous
	165 mg/kg	mouse	intravenous
	200 mg/kg	dog	oral
	200 mg/kg	dog	intravenous
	800 mg/kg	rabbit	oral
	100 mg/kg	rabbit	intravenous
	182 mg/kg	guinea pig	oral
LD_{Lo}	420 mg/kg	rat	intrapertioneal

Non-lethal Acute Effects:

Inhibition of prothromben formation
Capillary damage

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 0.1 mg/m^3

Other Chronic Effects:

m-Xylene

CHEMICAL NAME

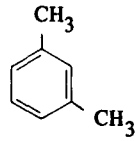
CAS Number: 108-38-3

Chemical Name: m-Xylene

Synonyms: m-Xylol

Molecular Formula: C_8H_{10}

Structure:



Chemical Properties

Molecular Weight: 106.2

Physical State: Liquid

Vapor Pressure: 8.56 mm at 25°C

Vapor Density: 3.66

Boiling Point: 139°C at 760 mm

Melting Point: -47.4°C

Density: 0.864 at 20°C/4°C

Solubility: Insoluble (0.13 gm/l H_2O)

Octanol/Water Partition Coefficient: 3.20

Environmental Persistence

BOD: Total theoretical oxygen demand = 3.17 gm/gm

Atmospheric Reactivity: Reacts with oxidizing materials

Activity toward O_3: $t_{1/2}$ = 100 years

RO_2: $t_{1/2}$ = 2200 years

OH: $t_{1/2}$ = 3 days

Common air contaminant, reported at 0.016 to 0.61 ppm

Safety Hazard:

Fire–dangerous

Explosion–moderate

PRODUCTION DATA

Annual U.S. Production: ca. 1710 x 10^6 lbs. (1975) (4907.1 x 10^6 lbs.-mixed xylenes, 1975)

Consumption: ca. 1710 x 10^6 lbs. (4907 x 10^6 lbs.-mixed xylenes)

Fraction of Dispersion: (0.13-mixed xylenes)

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): (ca. 765-mixed xylenes)

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	5000 mg/kg	rat	oral
LD_{Lo}	2000 mg/kg	rat	intraperitoneal
	5000 mg/kg	rat	subcutaneous
LC_{Lo}	8000 ppm (4 hours)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard: NIOSH recommended TWA 100 ppm

Carcinogenicity: Neoplastic effects in mice after dermal application

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:
- Anorexia
- CNS disturbances
- Hyperglycemia
- Leucopenia
- Leucocytosis
- Epidermal hypertrophy

o-Xylene

CHEMICAL NAME

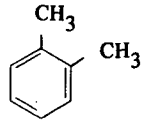
CAS Number: 95-47-6

Chemical Name: o-Xylene

Synonyms: o-Xylol

Molecular Formula: C_8H_{10}

Structure:



Chemical Properties

Molecular Weight: 106.2

Physical State: Liquid

Vapor Pressure: 10 mm at 32.1°C

Vapor Density:

Boiling Point: 144.4°C at 760 mm

Melting Point: -25°C

Density: 0.880 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient: 2.77

Environmental Persistence

BOD: Total theoretical oxygen demand = 3.17 gm/gm

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate
Explosion–slight

PRODUCTION DATA

Annual U.S. Production: 679.7 x 10^6 lbs. (1975)

Consumption: 679.7 x 10^6 lbs.

Fraction of Dispersion: (0.13-mixed xylenes)

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): (ca. 765-mixed xylenes)

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	5000 mg/kg	rat	oral
	1500 mg/kg	rat	intraperitoneal
	2500 mg/kg	mouse	subcutaneous
LC_{Lo}	6920 ppm	mouse	inhalation

Chronic Toxicity

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

Carcinogenicity: Neoplastic effects in mice after dermal applications

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Leucopenia and leucocytosis
CNS disturbances
Anorexia
Hyperglycemia
Epidermal hypertrophy

p-Xylene

CHEMICAL NAME

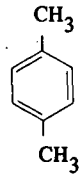
CAS Number: 106-42-3

Chemical Name: p-Xylene

Synonyms: p-Xylol

Molecular Formula: C_8H_{10}

Structure:



Chemical Properties

Molecular Weight: 106.2

Physical State: Liquid

Vapor Pressure: 10 mm at 27.3°C

Vapor Density: 3.66

Boiling Point: 138.5°C at 760 mm

Melting Point: 13.2°C

Density: 0.8611 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient: 3.15

Environmental Persistence

BOD: Total theoretical oxygen demand = 3.179 gm/gm

Atmospheric Reactivity: Reacts with oxidizing materials

Activity toward RO_2: $t_{1/2}$ = 2200 years

O_3: $t_{1/2}$ = 100 years

OH: $t_{1/2}$ = 3 days

Safety Hazard:

Fire–moderate

Explosion–moderate

PRODUCTION DATA

Annual U.S. Production: 2419.3 x 10^6 lbs. (1975)

Consumption: 2419.3 x 10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 39.9

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	5000 mg/kg	rat	oral
LD_{Lo}	2000 mg/kg	rat	intraperitoneal
	5000 mg/kg	rat	subcutaneous
LC_{Lo}	3460 ppm	mouse	inhalation

Chronic Toxicity

U.S. Occupational Standard: NIOSH recommended: TWA 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Leucopenia and leucocytosis
CNS disturbances
Anorexia
Hyperglycemia
Epidermal hypertrophy

Xylenesulfonic acid, sodium salt

CHEMICAL NAME

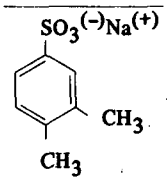
CAS Number: 827-93-0

Chemical Name: 3,4-Xylenesulfonic acid, sodium salt

Synonyms: Sodium xylene sulfonate

Molecular Formula: $C_8H_{10}O_3S \cdot Na$

Structure:



Chemical Properties

Molecular Weight: 209.23

Physical State:

Vapor Pressure: Negligible at 25°C

Vapor Density:

Boiling Point:

Melting Point:

Density:

Solubility:

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Xylenesulfonic acid, sodium salt

PRODUCTION DATA

Annual U.S. Production: 37.4 x 10^6 lbs.

Consumption: 37.4 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.3

Release Rate (million lbs/yr): 38.5

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	500 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

2, 6-Xylenol

CHEMICAL NAME

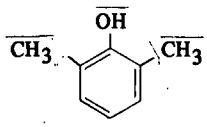
CAS Number: 576-26-1

Chemical Name: 2,6-Dimethylphenol

Synonyms: Xylenol

Molecular Formula: $C_8H_{10}O$

Structure:



Chemical Properties

Molecular Weight: 122.18

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 212°C at 760 mm

Melting Point: 49°C

Density: 0.984 at 60°C/15.5°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient: 2.33

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

2, 6-Xylenol

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}	296 mg/kg	rat	oral
	980 mg/kg	mouse	oral
	920 mg/kg	mouse	skin
	150 mg/kg	mouse	intraperitoneal
	700 mg/kg	rabbit	oral

Chronic Toxicity

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

Carcinogenicity:

Neoplastic effects:

TD_{Lo}	4000 mg/kg (120 weeks)	mouse	skin

Mutagenicity:

Teratogenicity:

TLV:
Odor perception: 200 ppm

Other Chronic Effects:

3, 5-Xylenol

CHEMICAL NAME

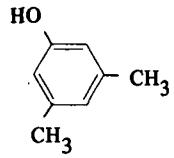
CAS Number: 1300-71-6

Chemical Name: Dimethylphenol

Synonyms: Xylenol
3,5-Xylenol
5-Hydroxy-1, 3-dimethylbenzene
3,5-Dimethylphenol
1-Hydroxy-3, 5-dimethylbenzene

Molecular Formula: $C_8H_{10}O$

Structure:



Chemical Properties

Molecular Weight: 122.17

Physical State: Solid

Vapor Pressure: 1 mm at 62.0°C

Vapor Density:

Boiling Point: 219.5°C (sublimes)

Melting Point: 68°C

Density: 0.9680 at 20°C/4°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 31% of theoretical

Atmospheric Reactivity:

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}	1070 mg/kg	mouse	oral
LD_{Lo}	1750 mg/kg	guinea pig	subcutaneous

Chronic Toxicity

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

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Zinc stearate

CHEMICAL NAME

CAS Number: 557-05-1

Chemical Name: Octadecanoic acid, zinc salt

Synonyms: Stearic acid, zinc salt

Molecular Formula: $(C_{18}H_{35}O_2)_2 \cdot Zn$

Structure: $[CH_3(CH_2)_{16}COO^-]_2 Zn^{2+}$

Chemical Properties

Molecular Weight: 632.30

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point:

Melting Point: 130°C

Density: 1.095

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–slight

PRODUCTION DATA

Annual U.S. Production: 19.4 x 10^6 lbs.

Consumption: 19.4 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 20.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Non-lethal Acute Effects:
Pulmonary fibrosis

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

CHEMICAL NAME INDEX

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(Please read Instructions on the reverse before completing)

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15. SUPPLEMENTARY NOTES

16. ABSTRACT

This is the fourth 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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