United States
Environmental Protection
Agency

Industrial Environmental Research
Laboratory
Research Triangle Park NC 27711

Research and Development

EPA-600/S2-81-002 May 1981

EPA

Project Summary

Response Factors of VOC Analyzers Calibrated with Methane for Selected Organic Chemicals

G. E. Brown, D. A. DuBose, W. R. Phillips, and G. E. Harris

This report presents a summary of the results of a laboratory study on the sensitivity of portable Volatile Organic Compound (VOC) analyzers to a variety of organic chemicals. This type of analyzer is commonly used in monitoring for fugitive emissions, with most previous work having been done on the Century Systems OVA-108, OVA-128, or the J.W. Bacharach TLV Sniffer. The OVA-108 and the TLV were chosen for testing in this study.

The sensitivity of the analyzer was characterized by a response factor, which was defined as the ratio of the actual chemical concentration to the observed instrument response. Bag samples of known concentration were prepared by introducing a measured weight (or volume) of the subject chemical into a Tedlar bag containing a known volume of hydrocarbon-free air.

Such response factors were determined for 168 organic chemicals at a minimum of three concentrations. These data points were fitted to a predictive model to allow estimation of the instrument response at any concentration. This summary report presents the coefficients of the predictive equation for each chemical as well as the fitted response factor at an actual concentration of 10,000 parts per million by volume (ppmv).

This Project Summary was developed by EPA's Industrial Environmental Research Laboratory in Research Triangle Park, N.C. to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

This report presents the results of a laboratory study on the sensitivity of two types of portable hydrocarbon detectors to a variety of organic chemicals. The introductory section briefly discusses the background, objectives, and procedures used in the project.

The study of fugitive VOC emissions has rapidly gained emphasis over the past several years. Several research efforts designed to measure fugitive emission levels and to assess the effectiveness of proposed control schemes are in various stages of completion. The development of regulations to control fugitive emissions has begun at both the State and Federal level.

As a result of this research, a roughly quantitative method for leak detection has been developed which is commonly called "screening." The screening process is simply the measurement of the VOC concentration at a point close

to the potential leak site (valve stem, pump seal, etc.). The measurement is made with a portable VOC detector. While many instruments could potentially be used for this service, the bulk of the existing data has been taken using either the J. W. Bacharach "TLV Sniffer," the Century Systems "OVA-108," or the "OVA-128."

While these instruments will respond to almost any combustible material, they exhibit different sensitivities to various types of hydrocarbons and substituted organic chemicals. The "response factor" is a correction factor which quantifies these differences in sensitivity.

The primary objective of this work was to experimentally determine the response factors for a large number of commonly encountered chemical species. Such response factors are presented here for both the OVA and the TLV. Two instruments of each type (one old and one new) were tested to check for instrument-to-instrument variations. Each chemical was tested at several concentrations to assess variations in the response factor over the range of interest.

The experimental determination of a response factor simply requires reading the observed concentration on the instrument when testing a gas sample of known concentration. The response factor is then calculated by:

$$\text{Response Factor (RF)} = \frac{\text{Actual Concentration}}{\text{Observed Concentration}}$$

The standard gas samples were prepared by one of two methods, depending on the volatility of the subject chemical. Liquids with low to medium volatility were injected into a Tedlar bag containing a measured volume of hydrocarbon-free air. The maximum concentration tested was limited to 90 percent of the saturated concentration at lab conditions to prevent condensation or incomplete vaporization. The chemical was injected with a microliter syringe, which was weighed before and after injection on an electronic balance to get a precise measure of the chemical introduced into the bag.

Standard gas mixtures for gases and highly volatile liquids were prepared volumetrically. A cylinder of standard gas was purchased at, or above, the highest concentration to be tested. Dilutions of this purchased gas with zero air were made on a manifold with the flows controlled by needle valves and the flowrate of each gas measured on bubble meters.

Response data were collected for 168 organic chemicals at a minimum of three concentrations each. The response factor of most of these chemicals varied significantly with concentration, which made it difficult to characterize the response of a chemical with a single figure. Accordingly, a correlation was developed between response and actual concentration that would estimate the response at any concentration. This predictive equation was used to generate a table of estimated response factors at 10,000 ppmv, as shown in Table 1.

The user can generate estimates of the response factor at any concentration by the following equation:

$$\text{Response Factor} = C/IR_c$$

$$IR_c = \exp(a + b \cdot \ln C + Se^2/2)$$

where IR_c is the instrument response to a concentration of "C" ppmv, and "a," "b" and "Se" are constants given for each chemical in Table 2 and Table 3 for the OVA and TLV, respectively. The 95 percent confidence intervals bounding this response factor estimate can be calculated by:

$$\ln(C_u) = \ln(IR_c) + t \cdot S_{IR}^c$$

$$\text{and } \ln(C_L) = \ln(IR_c) - t \cdot S_{IR}^c$$

where C_u is the upper confidence interval, C_L is the lower confidence interval, t is the tabulated student's t with N-2 degrees of freedom for 95 percent confidence, and

$$S_{IR}^c = \sqrt{S_e^2 \cdot [(1/n) + (\ln C - \bar{X})^2/SS_X}$$

where S_e, n, X, and SS_X are constants for each chemical given in Tables 2 and 3.

Conclusions

Response factors were determined at a minimum of three concentrations for 168 organic chemicals. The response factors of most of these compounds cannot be adequately represented by a single number, as they vary significantly with concentration. This report provides estimates of the response factors at a concentration of 10,000 ppmv, and a correlation to estimate response factors for other concentrations of interest.

Recommendations

The complete document provides a large body of data on the sensitivity of response of VOC analyzers, but much work is left to be done. All of the work reported here is on individual chemicals yet such pure streams are rare in the industrial processes which will be surveyed for fugitive emissions. Data on the response characteristics of chemical mixtures are essential to accurate field measurements. Further work could also be justified to try to develop a method to predict the response factor of chemicals not yet tested based on their functional groups and carbon numbers. This effort would probably be facilitated by the development of a mechanistic, rather than an empirical, model of response.

Table 1. *Fitted Response Factors with 95% Confidence Intervals, Estimated at 10,000 PPMV*

OCPDB* ID No	Compound Name	Volatility Class**	OVA Response Factor	OVA Confidence Intervals	TLV Response Factor	TLV Confidence Intervals
70	Acetic Acid	LL	1.83	(1.17- 2.87)	5.70	(4.16- 7.81)
80	Acetic Anhydride	LL	1.36	(1.12- 1.65)	2.89	(1.62- 5.14)
90	Acetone	LL	0.79	(0.53- 1.19)	1.22	(0.81- 1.83)
100	Acetone Cyanohydrin	HL	3.42	(0.70- 16.83)	7.84	(1.40- 43.78)
110	Acetonitrile	LL	0.94	(0.85- 1.05)	1.17	(0.96- 1.42)
120	Acetophenone	HL	10.98	(5.56- 21.68)	54.86	(38.35- 78.48)
125	Acetyl Chloride	LL	1.99	(1.76- 2.26)	2.59	(1.81- 3.71)

* *Organic Chemical Producers Data Base.*

** *G = Gas; LL = Light Liquid; HL = Heavy Liquid.*

Table 1. *(continued)*

OCPDB* ID No	Compound Name	Volatility Class**	OVA Response Factor	OVA Confidence Intervals	TLV Response Factor	TLV Confidence Intervals
-	Acetyl-1-Propanol, 3-	LL	10.87	(6.58- 17.95)	25.81	(13.70- 48.63)
130	Acetylene	G	0.37	(0.32- 0.43)	11.95	(10.41- 13.73)
160	Acrylic Acid	LL	4.65	(3.85- 5.61)	36.95	(5.34-255.69)
170	Acrylonitrile	LL	0.96	(0.79- 1.17)	2.70	(0.44- 16.36)
-	Allene	G	0.55	(0.49- 0.61)	5.78	(5.36- 6.24)
200	Allyl Alcohol	LL	0.94	(0.69- 1.30)		(-)
250	Amyl Alcohol, N-	HL	0.69	(0.47- 1.00)	1.78	(1.19- 2.66)
2855	Amylene	LL	0.31	(0.19- 0.51)	1.03	(0.46- 2.32)
330	Anisole	LL	0.92	(0.64- 1.32)	2.69	(1.69- 4.27)
360	Benzaldehyde	HL	2.36	(1.52- 3.68)	6.30	(5.77- 6.88)
380	Benzene	LL	0.21	(0.19- 0.24)	1.07	(0.97- 1.19)
450	Benzonitrile	HL	2.24	(1.18- 4.24)	9.13	(2.82- 29.62)
490	Benzoyl Chloride	HL	6.40	(3.20- 12.80)	6.60	(3.41- 12.79)
530	Benzyl Chloride	HL	4.23	(2.74- 6.52)	4.87	(2.50- 9.48)
570	Bromobenzene	LL	0.36	(0.28- 0.46)	1.16	(0.69- 1.94)
590	Butadiene, 1, 3-	G	0.37	(0.34- 0.42)	6.00	(5.64- 6.39)
-	Butane, N-	G	0.38	(0.31- 0.46)	0.68	(0.61- 0.75)
640	Butanol, N	LL	1.43	(0.66- 3.13)	2.80	(1.49- 5.27)
650	Butanol, Sec-	LL	0.70	(0.63- 0.78)	1.26	(1.00- 1.57)
660	Butanol, Tert	S	0.44	(0.26- 0.74)	2.19	(1.54- 3.11)
592	Butene, 1-	G	0.51	(0.45- 0.58)	2.97	(2.73- 3.24)
600	Butyl Acetate, N-	LL	0.60	(0.46- 0.78)	1.30	(1.18- 1.42)
630	Butyl Acrylate, N-	LL	0.64	(0.56- 0.74)	1.98	(0.89- 4.43)
-	Butyl Ether, N	LL	2.70	(1.95- 3.73)	2.66	(1.42- 4.95)
-	Butyl Ether, Sec	LL	0.26	(0.11- 0.60)	1.13	(0.78- 1.64)
670	Butylamine, N-	LL	0.63	(0.43- 0.92)	1.91	(1.38- 2.65)
680	Butylamine, Sec-	LL	0.67	(0.53- 0.84)	1.50	(1.26- 1.79)
690	Butylamine, Tert-	LL	0.58	(0.52- 0.65)	1.80	(1.53- 2.11)
-	Butylbenzene, Tert-	HL	1.27	(0.94- 1.73)	6.42	(1.82- 22.67)
750	Butyraldehyde, N-	LL	1.39	(1.12- 1.71)	1.89	(1.60- 2.23)
760	Butyric Acid	HL	0.74	(0.22- 2.52)	4.58	(2.39- 8.78)
780	Butyronitrile	LL	0.46	(0.31- 0.70)	1.33	(0.44- 3.99)
790	Carbon Disulfide	LL	571.92	(279.65-1169.7)	2.96	(2.62- 3.34)
810	Carbon Tetrachloride	LL	21.28	(10.95- 41.36)	30.52	(8.96-103.88)
830	Chloroacetaldehyde	LL	13.40	(9.85- 18.24)	5.07	(3.65- 7.06)
890	Chlorobenzene	LL	0.36	(0.28- 0.48)	0.88	(0.77- 1.00)
1740	Chloroethane	G	0.67	(0.02- 22.54)	2.16	(0.31- 14.95)
930	Chloroform	LL	4.48	(3.60- 5.56)	8.77	(5.65- 13.64)
960	Chlorophenol, O-	HL	3.33	(1.88- 5.92)	5.87	(2.45- 14.06)
-	Chloropropene, 1-	LL	0.59	(0.53- 0.66)	0.86	(0.64- 1.15)
210	Chloropropene, 3-	LL	0.75	(0.65- 0.87)	1.24	(1.09- 1.41)
970	Chlorotoluene, M-	LL	0.43	(0.39- 0.47)	0.92	(0.70- 1.21)
980	Chlorotoluene, O-	LL	0.45	(0.38- 0.54)	1.05	(0.70- 1.58)
990	Chlorotoluene, P-	LL	0.52	(0.47- 0.58)	1.15	(0.62- 2.12)
1010	Cresol, O-	S	0.95	(0.59- 1.52)	3.98	(0.22- 72.91)
1040	Crotonaldehyde	LL	1.32	(0.78- 2.23)	8.54	(2.33- 31.36)
1060	Cumene	LL	1.92	(1.13- 3.28)	12.49	(5.62- 27.74)
1120	Cyclohexane	LL	0.36	(0.26- 0.50)	0.72	(0.63- 0.82)
1130	Cyclohexanol	HL	0.82	(0.58- 1.17)	4.92	(1.18- 20.48)
1140	Cyclohexanone	LL	1.50	(1.01- 2.22)	3.99	(1.79- 8.91)
1150	Cyclohexene	LL	0.40	(0.32- 0.51)	1.84	(1.65- 2.05)
1160	Cyclohexylamine	LL	0.47	(0.28- 0.79)	1.38	(1.31- 1.45)
-	Decane	HL	0.00	(0.00- 3.31)	0.20	(0.00- 31.01)
1190	Diacetone Alcohol	HL	1.53	(1.01- 2.31)	0.98	(0.29- 3.36)
-	Diacetyl	LL	1.61	(1.31- 1.99)	2.81	(2.15- 3.67)

* Organic Chemical Producers Data Base.

**G = Gas; LL = Light Liquid; HL = Heavy Liquid; S = Solid.

Table 1. *(continued)*

OCPDB* ID No	Compound Name	Volatility Class**	OVA Response Factor	OVA Confidence Intervals	TLV Response Factor	TLV Confidence Intervals
-	Dichloro-1-Propanol, 2,3-	LL	61.51	(30.13-125.55)	34.34	(23.80- 49.55)
1270	Dichloro-1-Propene, 2,3-	LL	0.70	(0.47- 1.05)	1.62	(1.22- 2.14)
-	Dichloro-2-Propanol, 1,3-	LL	29.34	(17.42- 49.40)	18.63	(12.95- 26.82)
1215	Dichlorobenzene, M-	HL	0.66	(0.56- 0.78)	1.89	(1.37- 2.60)
1216	Dichlorobenzene, O-	HL	0.70	(0.48- 1.03)	1.22	(0.80- 1.86)
-	Dichloroethane, 1,1-	LL	0.77	(0.60- 0.98)	1.80	(1.58- 2.06)
1244	Dichloroethane, 1,2-	LL	0.95	(0.77- 1.18)	2.08	(1.73- 2.51)
1235	Dichloroethylene, Cis 1,2-	LL	1.31	(1.08- 1.58)	1.93	(1.02- 3.66)
1236	Dichloroethylene, Trans 1,2	LL	1.13	(0.99- 1.30)	1.86	(0.55- 6.29)
2620	Dichloromethane	LL	2.26	(1.94- 2.64)	3.63	(2.72- 4.84)
3110	Dichloropropane, 1,2-	LL	1.03	(0.82- 1.29)	1.80	(1.12- 2.89)
1440	Diisobutylene	LL	0.24	(0.17- 0.35)	1.39	(0.97- 2.01)
-	Diisopropyl Benzene, 1,3-	LL	9.43	(3.68- 24.18)	24.96	(6.07-102.67)
1870	Dimethoxy Ethane, 1,2-	LL	1.28	(0.57- 2.90)	1.43	(1.16- 1.75)
1490	Dimethylformamide, N,N-	LL	3.89	(3.11- 4.85)	2.95	(2.86- 3.03)
1495	Dimethylhydrazine, 1,1-	LL	1.04	(0.71- 1.52)	2.74	(1.61- 4.67)
-	Dimethylstyrene, 2,4-	LL	37.09	(25.75- 53.42)	78.06	(38.51-158.23)
1520	Dimethylsulfoxide	HL	0.00	(0.00-4300.8)	4.88	(1.41- 16.92)
1480	Dioxane	LL	1.58	(1.10- 2.28)	1.23	(1.07- 1.41)
1650	Epichlorohydrin	LL	1.72	(1.61- 1.83)	2.02	(1.84- 2.22)
-	Ethane	G	0.57	(0.26- 1.26)	0.73	(0.21- 2.52)
1660	Ethanol	LL	2.04	(1.83- 2.28)		(-)
1910	Ethoxy Ethanol, 2-	LL	1.68	(1.38- 2.06)	1.61	(1.42- 1.84)
1670	Ethyl Acetate	LL	0.84	(0.74- 0.94)	1.37	(1.08- 1.74)
1680	Ethyl Acetoacetate	HL	3.02	(1.98- 4.62)	3.13	(2.71- 3.63)
1690	Ethyl Acrylate	LL	0.72	(0.55- 0.93)		(-)
1750	Ethyl Chloroacetate	LL	1.97	(1.76- 2.21)	1.47	(0.97- 2.23)
1990	Ethyl Ether	LL	0.97	(0.73- 1.28)	1.11	(1.01- 1.23)
1710	Ethylbenzene	LL	0.70	(0.45- 1.09)	3.14	(1.43- 6.92)
1770	Ethylene	G	0.52	(0.39- 0.68)	1.49	(1.27- 1.74)
1980	Ethylene Oxide	G	2.72	(2.31- 3.20)	2.43	(1.92- 3.07)
1800	Ethylenediamine	LL	1.78	(1.39- 2.28)	2.46	(1.83- 3.32)
2060	Formic Acid	LL	34.87	(29.00- 41.94)	33.21	(16.78- 65.73)
1221	Freon 12	G	9.65	(6.99- 13.33)	11.83	(3.63- 38.59)
2073	Furfural	HL	7.96	(3.69- 17.15	10.01	(9.72- 10.31)
2105	Glycidol	LL	8.42	(5.14- 13.81)	5.23	(2.68- 10.22)
-	Heptane	LL	0.30	(0.12- 0.75)	0.75	(0.56- 1.00)
-	Hexane, N-	LL	0.31	(0.26- 0.36)	0.72	(0.65- 0.79)
-	Hexene, 1-	LL	0.39	(0.26- 0.58)	2.92	(0.86- 9.89)
-	Hydroxyacetone	LL	8.70	(6.51- 11.64)	9.34	(6.21- 14.06)
-	Isobutane	G	0.30	(0.09- 0.95)	0.61	(0.44- 0.86)
2200	Isobutylene	G	2.42	(1.01- 5.84)	6.33	(0.09-460.41)
2350	Isoprene	LL	0.48	(0.32- 0.72)		(-)
2360	Isopropanol	LL	0.90	(0.68- 1.18)	1.35	(0.98- 1.86)
2370	Isopropyl Acetate	LL	0.68	(0.58- 0.80)	1.25	(1.11- 1.40)
2390	Isopropyl Chloride	LL	0.62	(0.52- 0.73)	0.99	(0.81- 1.19)
-	Isovaleraldehyde	LL	0.55	(0.45- 0.66)	2.04	(1.19- 3.51)
2450	Mesityl Oxide	LL	1.12	(0.94- 1.33)	3.12	(1.68- 5.79)
-	Methacrolein	LL	1.27	(0.91- 1.77)	3.10	(1.65- 5.83)
2460	Methacrylic Acid	HL	0.71	(0.06- 7.84)	6.61	(0.37-116.80)
2500	Methanol	LL	5.69	(4.96- 6.52)	1.88	(1.62- 2.18)
1930	Methoxy-Ethanol, 2-	LL	2.70	(1.99- 3.67)	2.19	(1.85- 2.60)
2510	Methyl Acetate	LL	1.80	(1.55- 2.08)	1.76	(1.47- 2.12)
-	Methyl Acetylene	G	0.53	(0.50- 0.57)	3.92	(3.59- 4.29)
2560	Methyl Chloride	G	1.75	(1.44- 2.14)	2.45	(1.62- 3.73)

* *Organic Chemical Producers Data Base.*

***G = Gas; LL = Light Liquid; HL = Heavy Liquid; S = Solid.*

Table 1. *(continued)*

OCPDB* ID No	Compound Name	Volatility Class**	OVA Response Factor	OVA Confidence Intervals	TLV Response Factor	TLV Confidence Intervals
2640	Methyl Ethyl Ketone	LL	0.57	(0.40- 0.81)	1.12	(0.93- 1.35)
2645	Methyl Formate	LL	3.47	(2.87- 4.19)	1.93	(1.76- 2.11)
2665	Methyl Methacrylate	LL	0.99	(0.89- 1.10)	2.36	(1.54- 3.62)
2650	Methyl-2-Pentanol, 4-	LL	1.70	(1.33- 2.17)	1.94	(1.46- 2.58)
2660	Methyl-2-Pentanone, 4-	LL	0.49	(0.38- 0.64)	1.54	(1.22- 1.94)
-	Methyl-2,4-Pentanediol, 2-	LL	96.34	(72.63-127.80)	67.07	(36.31-123.87)
2550	Methyl-3-Butyn-2-ol, 2	LL	0.51	(0.32- 0.79)		(-)
-	Methylal	LL	1.46	(1.09- 1.96)	1.41	(1.23- 1.62)
2540	Methylaniline, N-	HL	4.13	(3.75- 4.54)	5.25	(0.99- 27.84)
2570	Methylcyclohexane	LL	0.38	(0.12- 1.16)	0.85	(0.67- 1.07)
-	Methylcyclohexene, 1-	LL	0.33	(0.24- 0.45)	2.22	(1.70- 2.91)
2670	Methylpentynol	LL	1.17	(0.71- 1.92)	2.82	(1.92- 4.14)
2690	Methylstyrene, A-	LL	10.24	(8.30- 12.63)	31.46	(16.08- 61.53)
1660	Monoethanolamine	LL	28.04	(6.39-123.04)	25.83	(11.82- 56.44)
2700	Morpholine	LL	0.92	(0.64- 1.32)	1.93	(0.36- 10.40)
2770	Nitrobenzene	HL	29.77	(3.92-226.03)	40.61	(4.68-352.68)
2790	Nitroethane	LL	1.40	(1.23- 1.59)	2.54	(1.60- 4.04)
2791	Nitromethane	LL	3.32	(3.03- 3.64)	5.25	(2.32- 11.86)
2795	Nitropropane	LL	1.06	(0.79- 1.42)	1.77	(1.22- 2.57)
-	Nonane-N	LL	1.62	(0.93- 2.81)	5.54	(2.82- 10.89)
-	Octane	LL	1.04	(0.88- 1.22)	2.08	(1.76- 2.46)
2851	Pentane	LL	0.42	(0.30- 0.58)	0.62	(0.55- 0.69)
2910	Phenol	S	11.75	(7.55- 18.29)	12.01	(3.57- 40.43)
-	Phenyl-2-Propanol, 2-	LL	89.56	(69.84-114.83)	76.57	(46.38-126.42)
2973	Picoline, 2-	LL	0.34	(0.27- 0.41)	1.17	(1.10- 1.25)
-	Propane	G	0.88	(0.10- 7.54)	0.63	(0.24- 1.64)
3063	Propionaldehyde	LL	1.19	(1.02- 1.39)	1.65	(1.16- 2.36)
3066	Propionic Acid	LL	1.34	(1.06- 1.69)	3.51	(0.90- 13.62)
3070	Propyl Alcohol	LL	0.91	(0.72- 1.15)	1.15	(1.41- 1.71)
-	Propylbenzene, N-	LL	0.44	(0.37- 0.53)	5.97	(0.33-108.71)
3090	Propylene	G	0.79	(0.39- 1.57)	2.80	(0.96- 8.20)
3120	Propylene Oxide	LL	0.80	(0.69- 0.93)	1.15	(0.68- 1.93)
3130	Pyridine	LL	0.41	(0.33- 0.51)	1.17	(1.03- 1.32)
3230	Styrene	LL	4.16	(3.68- 4.71)	36.83	(7.32-185.28)
3290	Tetrachloroethane, 1,1,1,2	LL	3.00	(1.27- 7.07)	6.52	(3.82- 11.11)
3291	Tetrachloroethane, 1,1,2,2	LL	6.06	(4.78- 7.68)	14.14	(8.51- 23.51)
2860	Tetrachloroethylene	LL	3.16	(1.92- 5.21)	11.46	(8.64- 15.20)
3349	Toluene	LL	0.33	(0.29- 0.38)	2.32	(0.79- 6.82)
3393	Trichlorobenzene, 1,2,4-	HL	1.35	(0.13- 14.00)	0.39	(0.10- 1.57)
3395	Trichloroethane, 1,1,1-	LL	0.79	(0.70- 0.89)	2.41	(1.96- 2.96)
3400	Trichloroethane, 1,1,2-	LL	1.26	(1.08- 1.47)	3.68	(3.05- 4.43)
3410	Trichloroethylene	LL	0.94	(0.81- 1.08)	3.35	(2.68- 4.19)
3420	Trichloropropane, 1,2,3-	LL	0.95	(0.54- 1.69)	2.23	(1.47- 3.40)
3450	Triethylamine	LL	0.46	(0.32- 0.67)	1.41	(1.03- 1.92)
3510	Vinyl Acetate	LL	1.31	(0.97- 1.76)	3.99	(1.49- 10.69)
3520	Vinyl Chloride	G	0.65	(0.50- 0.84)	1.10	(0.79- 1.55)
-	Vinyl Propionate	LL	0.94	(0.40- 2.23)	0.70	(0.02- 22.87)
3530	Vinylidene Chloride	LL	1.15	(0.86- 1.54)	2.38	(1.95- 2.90)
3570	Xylene, P-	LL	2.27	(1.87- 2.76)	5.35	(3.34- 8.58)
3550	Xylene, M-	LL	0.30	(0.25- 0.37)	3.56	(0.93- 13.64)
3560	Xylene, O-	LL	0.36	(0.16- 0.77)	1.40	(0.73- 2.70)

* *Organic Chemical Producers Data Base.*

***G = Gas; LL = Light Liquid; HL = Heavy Liquid; S = Solid.*

Table 2. Statistics for Computing Estimates and Confidence Intervals, Type-OVA

OCPDB* ID No	Compound Name	Volatility Class**	A	B	N	SE	SSX	XBAR
70	Acetic Acid	LL	-2.8754	1.22149	23	0.677209	94.0588	6.71835
80	Acetic Anhydride	LL	.375288	.925664	6	.0924492	8.75857	6.97689
90	Acetone	LL	-.42601	1.06086	14	0.44568	56.4432	6.73273
100	Acetone Cyanohydrin	HL	-1.0724	.980583	6	0.206338	1.07377	5.97147
110	Acetonitrile	LL	-.80987	1.09408	6	.0616236	12.5475	7.23366
120	Acetophenone	HL	-1.013	.817811	14	0.768287	62.071	6.71836
125	Acetyl Chloride	LL	-.36506	.964417	6	.0778431	14.6944	7.21322
—	Acetyl-1-Propanol,3-	LL	1.07586	.611782	12	0.476851	50.5077	6.46174
130	Acetylene	G	.485665	1.05433	6	.0377039	1.44015	7.44562
160	Acrylic Acid	LL	-1.627	1.0091	6	0.112184	11.9679	7.31447
170	Acrylonitrile	LL	-.57262	1.06539	6	0.118698	14.1474	7.2202
—	Allene	G	-2.8183	1.37155	6	.0573086	4.4727	7.88619
200	Allyl Alcohol	LL	-3.6	1.39534	6	0.192964	13.7776	7.22368
250	Amyl Alcohol,N-	HL	-2.3527	1.29529	6	0.131896	5.39958	6.68114
2855	Amylene	LL	-2.5916	1.40493	6	0.231679	8.23563	7.0079
330	Anisole	LL	.083984	.998552	6	0.166868	8.64685	6.92252
360	Benzaldehyde	HL	-.44202	.953919	6	0.114793	3.55556	6.34483
380	Benzene	LL	-.87171	1.26135	31	0.148218	51.4347	6.63953
450	Benzonitrile	HL	1.60572	.735434	12	0.226988	6.18285	6.08178
490	Benzoyl Chloride	HL	1.74643	.599652	6	0.410048	13.2587	7.18737
530	Benzyl Chloride	HL	2.76717	.528787	12	0.511603	21.483	8.00839
570	Bromobenzene	LL	-.04983	1.11651	6	0.11169	7.72926	6.8984
590	Butadiene,1,3-	G	-5.7128	1.72671	6	.0471682	3.14273	7.7553
—	Butane,N-	G	-2.9002	1.42036	10	0.130245	3.61904	8.06308
640	Butanol,N	LL	-.96371	1.06262	3	0.233069	6.0393	7.04506
650	Butanol,Sec-	LL	-2.4932	1.30867	6	.0571548	10.6652	7.1325
660	Butanol,Tert	S	-1.7618	1.27647	6	0.248874	8.58158	7.03513
592	Butene,1-	G	-.75886	1.15507	6	.0686523	4.98197	7.7713
600	Butyl Acetate,	LL	-1.5906	1.22728	6	0.149389	11.2932	7.15691
630	Butyl Acrylate,N-	LL	-1.6738	1.22939	6	.0703242	9.90051	7.02981
—	Butyl Ether,N	LL	-1.3459	1.03767	3	0.114048	6.2084	7.50326
—	Butyl Ether,Sec	LL	-1.2453	1.27583	4	0.286528	4.87663	7.17385
670	Butylamine,N-	LL	-2.0713	1.27286	6	0.212276	11.2392	7.13838
680	Butylamine,Sec-	LL	-.90586	1.1415	6	0.13293	12.27	7.15
690	Bytylamine,Tert-	LL	-1.2282	1.19206	6	.0627487	11.0874	7.17992
—	Butylbenzene,Tert-	HL	.985678	.864887	6	0.186581	13.8471	7.21205
750	Butyraldehyde N-	LL	-2.8809	1.27649	6	0.126596	12.3356	7.29208
760	Butyric Acid	HL	-2.9839	1.35542	6	0.143141	.946825	5.84132
780	Butyronitrile	LL	-.92245	1.18116	6	0.203173	9.07656	7.0786
790	Carbon Disulfide	LL	-2.1633	.535771	6	0.424013	12.8302	7.22315
810	Carbon Tetrachloride	LL	2.13296	.427673	6	0.400795	13.7915	7.20605
830	Chloroacetaldehyde	LL	-4.2311	1.17545	8	0.198182	12.6252	7.1765
890	Chlorobenzene	LL	.590851	1.04424	10	0.15665	11.8805	6.68244
1740	Chloroethane	G	1.32501	0.5541	8	2.52458	40.5528	6.09409
930	Chloroform	LL	1.50605	0.67282	6	0.132055	13.3425	7.26212
960	Chlorophenol,O-	HL	.679952	.793318	6	0.202122	5.50648	6.66217
—	Chloropropene, 1-	LL	-2.2549	1.30157	7	.0754264	12.5689	7.30057
210	Chloropropene, 3-	LL	-2.3441	1.2843	12	0.136945	52.1424	6.45557
970	Chlorotoluene,M-	LL	-.46281	1.14167	6	0.039029	7.74444	6.9301
980	Chlorotoluene,O-	LL	0.09082	1.07555	6	0.0746	7.74409	6.88833
990	Chlorotoluene,P-	LL	-.48446	1.12273	6	.0479559	7.70788	6.93231
1010	Cresol,O-	S	-4.3483	1.4774	6	0.111396	2.9799	6.30801
1040	Crotonaldehyde	LL	-2.5728	1.24273	8	0.351319	12.9835	7.24563
1060	Cumene	LL	-1.2383	1.04932	12	0.509365	51.1558	6.46426
1120	Cyclohexane	LL	-2.0872	1.33603	6	0.146801	7.77672	6.96164
1130	Cyclohexanol	HL	-2.0239	1.24055	6	0899117	3.57046	6.28751
1140	Cyclohexanone	LL	-.38416	.995445	6	0.205081	10.3796	7.06142

* Organic Chemical Producers Data Base.

**G = Gas; LL = Light Liquid; HL = Heavy Liquid; S = Solid.

Table 2. (Continued)

OCPDB* ID No	Compound Name	Volatility Class**	A	B	N	SE	SSX	XBAR
1150	Cyclohexene	LL	-1.4625	1.25627	7	0.125436	10.0889	7.13077
1160	Cyclohexylamine	LL	-2.4639	1.34576	6	0.267438	9.7518	7.07654
—	Decane	HL	-14.781	3.45409	6	0.906647	.701072	5.67254
1190	Diacetone Alcohol	HL	-1.7754	1.14617	6	0.109833	3.44138	6.4446
—	Diacetyl	LL	-1.5731	1.11652	12	0.204878	49.1017	6.60012
—	Dichloro-1-Propanol,2,3-	LL	-3.0521	.873976	6	0.432654	13.6007	7.23629
1270	Dichloro-1-Propene,2,3-	LL	-1.9415	1.24672	6	0.217292	11.2697	7.10441
—	Dichloro-2-Propanol,1,3-	LL	-.79172	0.70996	8	0.410248	15.4488	7.55474
1215	Dichlorobenzene,M-	HL	.986623	.937663	6	.0547674	5.4863	6.59837
1216	Dichlorobenzene,O-	HL	1.10876	.917648	6	.0947476	3.19816	6.33962
—	Dichloroethane,1,1-	LL	-.00758	1.02819	6	0.130716	10.5488	7.11116
1244	Dichloroethane,1,2-	LL	-.30622	1.03745	6	0.131104	14.1446	7.2661
1235	Dichloroethylene,CIS1,2-	LL	-1.4618	1.12855	8	0.15056	15.325	7.54257
1236	Dichloroethylene,Trans1,2	LL	-2.0185	1.20515	8	.0862401	13.1057	7.02025
2620	Dichloromethane	LL	1.0934	.792123	6	.0915693	13.1072	7.23499
3110	Dichloropropane,1,2-	LL	-.88505	1.09215	6	0.123334	10.8605	7.1272
1440	Diisobutylene	LL	-2.0148	1.37176	6	0.165233	7.56692	6.9367
—	Diisopropyl Benzene,1,3-	LL	1.76459	.547649	6	0.561958	28.5679	6.27642
1870	Dimethoxy Ethane,1,2-	LL	-2.536	1.23573	6	0.483998	13.2176	7.19222
1490	Dimethylformamide,N,N-	LL	-.87643	.947127	6	0.109855	9.19596	7.02873
1495	Dimethylhydrazine 1,1-	LL	-3.7531	1.40074	6	0.230674	13.1967	7.26392
—	Dimethylstyrene,2,4-	LL	-1.5367	.771785	6	0.224922	13.6858	7.28067
1520	Dimethylsulfoxide	HL	-16.573	3.43902	6	1.0935	.409881	5.66978
1480	Dioxane	LL	-2.0521	1.17043	6	0.215831	13.0262	7.20306
1650	Epichlorohydrin	LL	-.75538	1.02334	6	.0376406	13.356	7.22066
—	Ethane	G	-2.0456	1.27648	6	0.325301	2.31961	7.84885
1660	Ethanol	LL	-2.9244	1.23973	6	0.068237	15.4173	7.19679
1910	Ethoxy Ethanol,2-	LL	-2.3344	1.19637	6	0.101094	9.75276	7.00472
1670	Ethyl Acetate	LL	-1.2288	1.15152	18	0.15158	66.2747	6.71408
1680	Ethyl Acetoacetate	HL	.494514	.825583	6	0.107831	3.5444	6.29103
1690	Ethyl Acrylate	LL	-2.1188	1.26487	6	0.144331	11.6226	7.14221
1750	Ethyl Chloroacetate	LL	-.60685	0.99184	6	.0551139	8.85726	6.99629
1990	Ethyl Ether	LL	-1.8661	1.20484	6	0.155052	11.6344	7.12129
1710	Ethylbenzene	LL	-1.0274	1.13086	20	0.597093	66.947	6.80288
1770	Ethylene	G	-8.0566	1.94541	6	0.157469	3.84623	8.01344
1980	Ethylene Oxide	G	-1.9953	1.10758	6	0.102798	4.79615	8.11482
1800	Ethylenediamine	LL	-1.0209	1.04732	6	0.146117	12.4844	7.23272
2060	Formic Acid	LL	-6.6759	1.33858	6	0.107919	12.0961	7.24228
1221	Freon 12	G	1.31433	.609471	6	0.174541	7.09205	7.51936
2073	Furfural	HL	1.04653	.650043	6	0.452342	12.6998	7.21469
2105	Glycidol	LL	-3.1147	1.10534	6	0.163724	4.78354	6.66621
—	Heptane	LL	-1.8365	1.32734	3	0.223944	3.74967	6.98098
—	Hexane,N-	LL	-1.7626	1.31685	37	0.199415	40.4766	6.87982
—	Hexene,1-	LL	-2.1275	1.33237	6	0.179963	7.54485	6.94449
—	Hydroxyacetone	LL	-3.2967	1.12007	8	0.232517	15.5756	7.59178
—	Isobutane	G	-2.2393	1.35824	8	0.557399	2.43992	7.90812
2200	Isobutylene	G	1.16949	.775741	6	0.147294	2.43034	5.46695
2350	Isoprene	LL	-2.8398	1.38474	6	0.215396	10.3612	7.11844
2360	Isopropanol	LL	-1.9189	1.21872	6	0.166719	13.4625	7.20498
2370	Isopropyl Acetate	LL	-.80703	1.12898	6	.0896555	12.0222	7.11716
2390	Isopropyl Chloride	LL	-1.6028	1.22527	8	0.127767	14.9689	7.52885
—	Isovaleraldehyde	LL	-2.7791	1.36676	6	0.102188	11.1909	7.14904
2450	Mesityl Oxide	LL	-2.5944	1.26898	6	0.10352	12.9133	7.1985
—	Methacrolein	LL	-2.8695	1.28287	6	0.233299	12.6663	7.72282
2460	Methacrylic Acid	HL	-6.6118	1.74781	6	0.366906	1.37953	6.10761
2500	Methanol	LL	-2.3981	1.06519	48	0.345716	185.666	7.35637
1930	Methoxy-Ethanol,2-	LL	-3.127	1.22972	6	0.181911	13.4296	7.2025

* *Organic Chemical Producers Data Base.*

**G = Gas; LL = Light Liquid; HL = Heavy Liquid; S = Solid.

Table 2. *(Continued)*

OCPDB* ID No	Compound Name	Volatility Class**	A	B	N	SE	SSX	XBAR
2510	Methyl Acetate	LL	-1.1087	1.0562	6	.0881283	12.9204	7.26467
—	Methyl Acetylene	G	-1.8489	1.26873	6	.0333733	3.13703	7.8821
2560	Methyl Chloride	G	-5.5539	1.54125	6	0.124856	3.89091	8.21681
2640	Methyl Ethyl Ketone	LL	-1.8876	1.26262	9	0.243063	25.2199	6.54915
2645	Methyl Formate	LL	-2.1378	1.09632	6	0.123123	16.9883	7.23917
2665	Methyl Methacrylate	LL	-1.8063	1.19693	6	.0609566	12.9869	7.19995
2650	Methyl-2-Pentanol,4-	LL	-0.916	1.03982	8	0.196403	15.6961	7.57994
2660	Methyl-2-Pentanone,4-	LL	-1.3252	1.22039	6	0.135332	10.2416	7.05588
—	Methyl-2,4-Pentanediol,2-	LL	-.20173	.524322	6	0.17221	13.1088	7.288
2550	Methyl-3-Butyn-2-OL,2	LL	-1.8974	1.27675	6	0.232082	10.1905	7.05895
—	Methylal	LL	-2.2406	1.19782	12	0.281975	52.6838	6.41101
2540	Methylaniline,N-	HL	-.71359	.923574	6	.0227449	3.11941	6.24884
2570	Methylcyclohexane	LL	-2.3663	1.34952	6	0.494885	7.87591	6.87425
—	Methylcyclohexene,1-	LL	-2.1159	1.34919	6	0.153802	8.95789	6.98327
2670	Methylpentynol	LL	-.06858	.985905	6	0.289271	12.5573	7.19601
2690	Methylstyrene, A-	LL	-1.2874	.884034	14	0.240239	66.6129	6.69408
1660	Monoethanolamine	LL	-2.4791	.855164	10	0.979098	22.2589	6.38433
2700	Morpholine	LL	-0.9405	1.10892	6	0.215556	13.3896	7.18013
2770	Nitrobenzene	HL	3.37879	.255857	5	0.403458	3.7675	5.51561
2790	Nitroethane	LL	-.38829	1.00525	6	.0769128	14.102	7.17721
2791	Nitromethane	LL	-.77951	.954076	6	.0563271	13.5221	7.27112
2795	Nitropropane	LL	-1.043	1.10518	6	0.179594	13.5435	7.26298
—	Nonane-N	LL	-1.5826	1.10603	14	0.501526	41.1309	6.3957
—	Octane	LL	-1.9407	1.20639	6	.0908505	11.4258	7.14769
2851	Pentane	LL	-2.059	1.31598	6	0.165283	9.68585	7.05094
2910	Phenol	S	.710164	.654066	10	0.155352	7.92326	5.72457
—	Phenyl-2-Propanol,2-	LL	1.00078	.402044	6	0.151805	13.1932	7.2875
2973	Picoline,2-	LL	-1.7278	1.30562	6	0.100047	8.91213	7.02075
—	Propane	G	0.76145	.882834	10	0.949772	3.20321	7.48077
3063	Propionaldehyde	LL	-2.8873	1.29443	6	.0929661	12.9242	7.24108
3066	Propionic Acid	LL	-1.4915	1.12963	6	.0994827	7.43093	6.89446
3070	Propyl Alcohol	LL	-2.4137	1.27078	6	0.142748	14.0456	7.22723
—	Propylbenzene,N-	LL	-1.2593	1.22527	6	.0785943	7.78882	6.93443
3090	Propylene	G	.864818	.926563	6	0.321062	4.94104	7.47693
3120	Propylene Oxide	LL	-1.5249	1.1886	7	0.103767	13.6953	7.43403
3130	Pyridine	LL	-.59723	1.16018	6	.0990446	8.47388	6.97017
3230	Styrene	LL	-1.3382	.990213	6	.0751161	13.777	7.23935
3290	Tetrachloroethane, 1,1,1,2	LL	1.50932	.697932	10	0.589679	17.5221	6.82617
3291	Tetrachloroethane,1,1,2,2	LL	-.63198	.872029	8	0.137087	12.074	6.91454
3349	Tetrachloroethylene	LL	-2.0129	1.05606	26	0.831676	113.842	6.77884
3349	Toluene	LL	-.55953	1.18126	6	.0633951	8.59474	6.8929
3393	Trichlorobenzene,1,2,4-	HL	-.17734	.982448	3	0.265473	1.23926	6.19843
3395	Trichloroethane,1,1,1-	LL	-.58382	1.08916	6	.0701193	12.7084	7.19096
3400	Trichloroethane,1,1,2-	LL	-.78558	1.05963	6	.0916246	12.8405	7.20735
3410	Trichloroethylene	LL	-1.6403	1.18484	6	.0879318	13.453	7.21675
3420	Trichloropropane,1,2,3-	LL	-2.9814	1.32332	6	0.31741	7.54119	7.5340
3450	Triethylamine	LL	-.68947	1.15664	6	0.17419	9.19563	6.95765
3510	Vinyl Acetate	LL	-1.4414	1.12549	6	0.178741	13.2953	7.2383
3520	Vinyl Chloride	G	-12.813	2.43718	3	.0838916	2.44541	8.0016
—	Vinyl Propionate	LL	-0.9365	1.10343	3	0.286336	6.59355	7.2926
3530	Vinylidene Chloride	LL	-2.3696	1.24041	6	0.172576	11.489	7.3405
3570	Xylene, P-	LL	-1.6901	1.09082	18	0.264759	76.5381	6.7331
3550	Xylene,M-	LL	-1.758	1.32044	6	0.084293	7.86889	6.885
3560	Xylene,O-	LL	-1.2606	1.24282	6	0.340035	7.74549	6.884

* *Organic Chemical Producers Data Base.*

***G = Gas; LL = Light Liquid; HL = Heavy Liquid; S = Solid.*

Table 3. Statistics for Computing Estimates and Confidence Intervals, Type-TLV

OCPDB* ID No	Compound Name	Volatility Class**	A	B	N	SE	SSX	XBAR
70	Acetic Acid	LL	1.53532	.633431	20	0.446849	81.6063	6.75306
80	Acetic Anhydride	LL	2.64396	.596488	3	0.149324	4.37929	6.97689
90	Acetone	LL	-.22007	.991616	14	0.452099	56.4432	6.73273
100	Acetone Cyanohydrin	HL	.900022	0.67604	6	0.222799	1.07377	5.97147
110	Acetonitrile	LL	.206418	.959987	6	0.113292	12.5475	7.23366
120	Acetophenone	HL	1.57858	.384909	14	0.40411	62.071	6.71836
125	Acetyl Chloride	LL	-.53649	0.95225	6	0.221368	14.6944	7.21322
—	Acetyl-1-Propanol,3-	LL	1.85273	.426187	12	0.60199	50.5077	6.46174
130	Acetylene	G	2.77721	.428709	5	.0808672	4.9029	8.1201
160	Acrylic Acid	LL	3.0261	.207029	6	1.15552	11.9679	7.31447
170	Acrylonitrile	LL	1.08345	0.70882	6	1.10159	14.1474	7.2202
—	Allene	G	1.48948	.647644	4	.0420336	4.48003	8.31859
250	Amyl Alcohol,N-	HL	1.69081	.753762	3	.0770913	2.69979	6.68114
2855	Amylene	LL	-2.7517	1.27023	9	0.679982	15.1755	7.62642
330	Anisole	LL	1.5387	0.72482	3	0.1171	4.32343	6.92252
360	Benzaldehyde	HL	2.73967	.502696	3	.0123884	1.77778	6.34483
380	Benzene	LL	0.28303	.960989	28	0.128504	55.3541	6.61165
450	Benzonitrile	HL	3.30419	.397316	6	0.263045	3.09142	6.08178
490	Benzoyl Chloride	HL	2.87184	0.48077	3	0.213308	6.62934	7.18737
530	Benzyl Chloride	HL	3.46699	.438342	6	0.495549	10.7415	8.00839
570	Bromobenzene	LL	1.40637	.830522	3	0.12348	3.86463	6.8984
590	Butadiene,1,3-	G	.498448	.751221	4	.0321868	4.16748	8.22042
—	Butane,N-	G	1.74095	.852814	7	.0692898	3.32684	8.337
640	Butanol,N	LL	1.36408	.738053	3	0.188523	6.0393	7.04506
650	Butanol,Sec-	LL	-.32886	1.00927	8	0.180589	15.8209	7.59599
660	Butanol,Tert	S	-.90524	1.01084	5	0.202464	8.24512	7.75919
592	Butene,1-	G	2.4338	.617307	5	.0537661	4.64345	8.27484
600	Butyl Acetate,	LL	1.47233	.811784	4	.0440696	8.27958	7.62533
630	Butyl Acrylate,N-	LL	1.69695	.738919	3	0.222439	4.95025	7.02981
—	Butyl Ether,N	LL	.973474	0.78565	3	0.218728	6.2084	7.50326
—	Butyl Ether,Sec	LL	.854386	.890522	6	0.242698	8.93521	7.78741
670	Butylamine,N-	LL	.058361	.921838	4	0.155349	8.07529	7.59075
680	Butylamine,Sec-	LL	.364395	.916162	3	.0543876	6.13498	7.15
690	Butylamine,Tert-	LL	.514191	.880031	4	0.076921	8.00765	7.63305
—	Butylbenzene,Tert-	HL	2.31474	.515112	6	0.763323	13.8471	7.21205
750	Butyraldehyde N-	LL	1.53293	0.76441	3	0.547613	6.1678	7.29208
760	Butyric Acid	HL	1.90498	.627895	3	.0415519	.473413	5.84132
780	Butyronitrile	LL	.400785	.919176	3	0.345687	5.88803	7.22597
790	Carbon Disulfide	LL	.809447	.794289	3	0.038928	6.41512	7.22315
810	Carbon Tetrachloride	LL	4.65946	.093298	6	0.738964	13.7915	7.20605
830	Chloroacetaldehyde	LL	-1.6493	1.00029	8	0.21254	12.6252	7.1765
890	Chlorobenzene	LL	.337457	.976794	11	0.116228	20.2555	7.35836
1740	Chloroethane	G	2.43057	.548012	8	1.38856	40.5528	6.09409
930	Chloroform	LL	1.1337	.637191	6	0.267978	13.3425	7.26212
960	Chlorophenol,O-	HL	1.99922	.589287	3	0.167483	2.75324	6.66217
—	Chloropropene, 1-	LL	-1.2944	1.15423	8	0.239914	16.3457	7.58835
210	Chloropropene, 3-	LL	-.29344	1.00783	12	0.123718	52.1424	6.45557
970	Chlorotoluene,M-	LL	.974584	.902659	3	.0661162	3.87222	6.9301
980	Chlorotoluene,O-	LL	1.12209	.871937	3	.095194	3.87205	6.88833
990	Chlorotoluene,P-	LL	.643704	.914041	3	0.149187	3.85394	6.93231
1010	Cresol,O-	S	2.24855	.598375	3	0.373867	1.48995	6.30801
1040	Crotonaldehyde	LL	2.10615	0.49768	8	0.866604	12.9835	7.24563
1060	Cumene	LL	.372112	.653917	12	0.762507	51.1558	6.46426
1120	Cyclohexane	LL	1.02342	.924071	10	0.119838	15.7682	7.68236
1130	Cyclohexanol	HL	3.00453	0.49349	6	0.363684	3.57046	6.28751
1140	Cyclohexanone	LL	1.20283	.709531	6	0.419218	10.3796	7.06142
1150	Cyclohexene	LL	1.36081	.785839	6	0734484	9.15524	7.81843

* Organic Chemical Producers Data Base.

**G = Gas; LL = Light Liquid; HL = Heavy Liquid; S = Solid.

Table 3. (Continued)

OCPDB* ID No	Compound Name	Volatility Class**	A	B	N	SE	SSX	XBAR
1160	Cyclohexylamine	LL	-.39214	1.00749	5	.0315026	8.99739	7.81516
—	Decane	HL	-3.6251	1.55525	6	0.484709	.701072	5.67254
1190	Diacetone Alcohol	HL	-2.3153	1.24765	6	0.324757	3.44138	6.4446
—	Diacetyl	LL	0.13275	.869795	12	0.259957	49.1017	6.60012
—	Dichloro-1-Propanol,2,3-	LL	2.70208	.319956	6	0.222292	13.6007	7.23629
1270	Dichloro-1-Propene,2,3-	LL	.779298	.861583	5	0.169488	9.26572	7.79473
—	Dichloro-2-Propanol,1,3-	LL	.358175	.639059	8	0.286746	15.4488	7.55474
1215	Dichlorobenzene,M-	HL	1.75138	.740694	3	.0598515	2.74315	6.59837
1216	Dichlorobenzene,O-	HL	1.02702	.866847	3	.0570792	1.59908	6.33962
—	Dichloroethane,1,1-	LL	-.15658	.952456	8	0.105846	15.7135	7.57506
1244	Dichloroethane,1,2-	LL	-.34562	.957124	6	0.116586	14.1446	7.2661
1235	Dichloroethylene,CIS1,2-	LL	-3.9143	1.33988	8	0.500384	15.325	7.54257
1236	Dichloroethylene,Trans1,2	LL	-2.9985	1.22745	8	0.752501	13.1057	7.02025
2620	Dichloromethane	LL	-.89162	.955286	6	0.173045	13.1072	7.23499
3110	Dichloropropane,1,2-	LL	-2.2472	1.17229	8	0.380407	15.8547	7.58337
1440	Diisobutylene	LL	-.09895	.969107	10	0.318329	15.3066	7.62355
—	Diisopropyl Benzene,1,3-	LL	2.06897	.387379	6	0.843952	28.5679	6.27642
1870	Dimethoxy Ethane,1,2-	LL	1.0292	.849491	3	.0667093	6.60878	7.19222
1490	Dimethylformamide,N,N-	LL	2.15791	.648372	3	.0077422	4.59798	7.02873
1495	Dimethylhydrazine 1,1-	LL	-1.1679	1.01568	3	0.17593	6.59834	7.26392
—	Dimethylstyrene,2,4-	LL	1.84209	.316572	6	0.435465	13.6858	7.28067
1520	Dimethylsulfoxide	HL	1.19045	.698461	3	0.049848	.204941	5.66978
1480	Dioxane	LL	1.90645	.770596	3	.0435575	6.5131	7.20306
1650	Epichlorohydrin	LL	-.63762	.992733	6	.0562992	13.356	7.22066
—	Ethane	G	1.67058	.849183	3	0.28197	1.15981	7.84885
1910	Ethoxy Ethanol,2-	LL	1.38151	.798001	3	.0354359	4.87638	7.00472
1670	Ethyl Acetate	LL	.671462	.887545	18	0.309859	66.2747	6.71408
1680	Ethyl Acetoacetate	HL	1.96467	0.66266	3	.0202922	1.7722	6.29103
1750	Ethyl Chloroacetate	LL	1.10037	.837749	3	0.108622	4.42863	6.99629
1990	Ethyl Ether	LL	1.60083	.814314	4	.0494937	8.56318	7.59965
1710	Ethylbenzene	LL	.665875	.735578	19	1.11767	68.9211	6.97741
1770	Ethylene	G	.594303	.891134	6	0.145849	6.26961	8.8141
1980	Ethylene Oxide	G	-1.0089	1.01284	3	.0811012	2.39808	8.11482
1800	Ethylenediamine	LL	1.26645	.764087	3	.0956445	6.24219	7.23272
2060	Formic Acid	LL	-.27968	.641373	6	0.39944	12.0961	7.24228
1221	Freon 12	G	.067945	.702149	6	0.639168	7.09205	7.51936
2073	Furfural	HL	2.48411	.480107	3	.0094205	6.34988	7.21469
2105	Glycidol	LL	-1.2608	.954506	6	0.221402	4.78354	6.66621
—	Heptane	LL	.990665	0.92378	3	.0713575	3.74967	6.98098
—	Hexane,N-	LL	1.36541	.886527	26	0.126527	35.4753	7.23407
—	Hexene,1-	LL	1.17156	0.6936	10	1.07612	15.3057	7.65326
—	Hydroxyacetone	LL	-.64006	.821067	8	0.326534	15.5756	7.59178
—	Isobutane	G	2.21202	.809978	7	0.236544	4.02085	8.25287
2200	Isobutylene	G	2.47459	.502984	6	0.71852	2.43034	5.46695
2360	Isopropanol	LL	.450358	.916636	6	0.192117	13.4625	7.20498
2370	Isopropyl Acetate	LL	1.49877	.813083	4	.0570508	8.54523	7.5767
2390	Isopropyl Chloride	LL	-.24062	1.02655	8	0.148871	14.9689	7.52885
—	Isovaleraldehyde	LL	.012977	.910504	8	0.438335	16.1261	7.60251
2450	Mesityl Oxide	LL	-1.1452	.993585	6	0.363946	12.9133	7.1985
—	Methacrolein	LL	-.47037	.905636	8	0.643145	18.2865	8.20673
2460	Methacrylic Acid	HL	-.69002	0.85944	6	0.438606	1.37953	6.10761
2500	Methanol	LL	.181625	.906937	32	0.296364	119.802	7.24719
1930	Methoxy-Ethanol,2-	LL	2.07507	.689261	3	.0552239	6.7148	7.2025
2510	Methyl Acetate	LL	.165303	.919727	6	0.109923	12.9204	7.26467
—	Methyl Acetylene	G	1.26462	.714083	5	.0537374	3.42491	8.3449
2560	Methyl Chloride	G	-5.2929	1.47615	3	0.143325	1.94546	8.21681
2640	Methyl Ethyl Ketone	LL	-.26525	1.01477	11	0.178905	35.5776	7.00659

* *Organic Chemical Producers Data Base.*

**G = Gas; LL = Light Liquid; HL = Heavy Liquid; S = Solid.

Table 3. (Continued)

OCPDB* ID No	Compound Name	Volatility Class**	A	B	N	SE	SSX	XBAR
2645	Methyl Formate	LL	-.54896	.988267	6	.0582411	16.9883	7.23917
2665	Methyl Methacrylate	LL	-.61443	.970127	6	0.252803	12.9869	7.19995
2650	Methyl-2-Pentanol,4-	LL	-.32448	.960325	8	0.227184	15.6961	7.57994
2660	Methyl-2-Pentanone,4-	LL	0.64249	.880799	10	0.222826	18.0426	7.77479
—	Methyl-2,4-Pentanediol,2-	LL	1.40603	.383098	6	0.373948	13.1088	7.288
—	Methylal	LL	.426532	.915145	12	0.131833	52.6838	6.41101
2540	Methylanilene,N-	HL	1.45363	.659612	3	0.214953	1.55971	6.24884
2570	Methylcyclohexane	LL	.270354	.986468	10	0.209975	16.6993	7.63536
—	Methylcyclohexene,1-	LL	1.20211	.779284	10	0.253704	17.4672	7.72897
2670	Methylpentynol	LL	.378822	.843633	6	0.224115	12.5573	7.19601
2690	Methylstyrene, A-	LL	1.5176	.428728	14	0.768371	66.6129	6.69408
1660	Monoethanolamine	LL	3.77579	.231518	5	0.317533	11.1294	6.38433
2700	Morpholine	LL	.417395	.867233	3	0.543624	6.69482	7.18013
2770	Nitrobenzene	HL	5.86537	-.04625	4	0.364955	2.79181	5.73648
2790	Nitroethane	LL	1.30098	.753164	6	0.278354	14.102	7.17721
2791	Nitromethane	LL	-.09862	.817192	6	0.498902	13.5221	7.27112
2795	Nitropropane	LL	1.14653	.810834	6	0.22734	13.5435	7.26298
—	Nonane-N	LL	.745275	.712676	14	0.614029	41.1309	6.3957
—	Octane	LL	-.54983	.979727	6	.0939152	11.4258	7.14769
2851	Pentane	LL	.069793	1.04455	8	.0904502	15.1917	7.52991
2910	Phenol	S	2.83764	.418267	5	0.261277	3.96163	5.72457
—	Phenyl-2-Propanol,2-	LL	2.79853	0.22002	6	0.306155	13.1932	7.2875
2973	Picoline, 2-	LL	.044869	.977725	5	.0380285	8.34831	7.73468
—	Propane	G	1.40707	.875637	7	0.632665	5.85865	7.95726
3063	Propionaldehyde	LL	.034692	.938077	7	0.260854	15.4002	7.48396
3066	Propionic Acid	LL	.705684	.772068	5	0.526247	7.1852	6.80396
3070	Propyl Alcohol	LL	1.48397	.791088	3	.0321125	7.0228	7.22723
—	Propylbenzene,N-	LL	2.15539	.480363	6	1.29885	7.78882	6.93443
3090	Propylene	G	3.54911	.466641	8	0.815257	8.85238	7.88063
3120	Propylene Oxide	LL	-.10224	.989086	7	0.366882	14.1261	7.45571
3130	Pyridine	LL	-.24347	1.00886	12	0.130339	18.0116	7.85092
3230	Styrene	LL	1.92813	.346454	6	0.984542	13.777	7.23935
3290	Tetrachloroethane,1,1,1,2	LL	-1.6641	.969855	10	0.367616	17.5221	6.82611
3291	Tetrachloroethane,1,1,2,2	LL	-1.0205	0.81849	8	0.293543	12.074	6.91454
2860	Tetrachloroethylene	LL	0.31901	.688569	26	0.469724	113.842	6.77884
3349	Toluene	LL	.120702	.851475	9	0.901616	16.2675	7.5501
3393	Trichlorobenzene,1,2,4-	HL	-1.3223	1.24323	3	0.1571	1.23926	6.19842
3395	Trichloroethane,1,1,1-	LL	-.92319	1.00391	6	0.120871	12.7084	7.19098
3400	Trichloroethane,1,1,2-	LL	-1.2924	0.99825	6	0.1101	12.8405	7.20735
3410	Trichloroethylene	LL	-.14259	.883197	6	0.134591	13.453	7.21675
3420	Trichloropropane,1,2,3-	LL	-2.3703	1.16714	6	0.233901	7.54119	7.53407
3450	Triethylamine	LL	.797863	.874591	5	0.180692	8.96445	7.71796
3510	Vinyl Acetate	LL	0.47409	.779072	6	0.593492	13.2953	7.23837
3520	Vinyl Chloride	G	-7.0574	1.75493	3	0.110247	2.44541	8.00167
—	Vinyl Propionate	LL	-11.761	2.24221	3	1.16066	6.59355	7.29263
3530	Vinylidene Chloride	LL	-.75599	.987246	6	0.117839	11.489	7.34056
3570	Xylene, P-	LL	-.13472	.813054	17	0.597877	70.8015	6.59625
3550	Xylene,M-	LL	.644307	.716846	10	1.17881	15.9403	7.60576
3560	Xylene,O-	LL	-.54235	1.01815	4	0.266544	6.46294	7.3494

* Organic Chemical Producers Data Base.

**G = Gas; LL = Light Liquid; HL = Heavy Liquid; S = Solid.

☆ U.S. GOVERNMENT PRINTING OFFICE 1981 -757-012/7115

G. E. Brown, D. A. DuBose, W. R. Phillips, and G. E. Harris are with Radian Corporation, Austin, TX 78759.
***Bruce A. Tichenor** is the EPA Project Officer (see below).*
The complete report, entitled "Response Factors of VOC Analyzers Calibrated with Methane for Selected Organic Chemicals," (Order No. PB 81-136 194; Cost: $30.50, subject to change) will be available only from:
National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650
The EPA Project Officer can be contacted at:
Industrial Environmental Research Laboratory
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711

United States
Environmental Protection
Agency

Center for Environmental Research
Information
Cincinnati OH 45268

Postage and
Fees Paid
Environmental
Protection
Agency
EPA 335

Official Business
Penalty for Private Use $300

RETURN POSTAGE GUARANTEED

PS 0000329
U S ENVIR PROTECTION AGENCY
REGION 5 LIBRARY
230 S DEARBORN STREET
CHICAGO IL 60604