

Table of compounds for ASI-1 (Drs. Farrington and Reddy)

Halogenated solvents and other volatile organic compounds

Compound name	Mol. Formula	Structure	Mol. Weight	Water Sol. (mol L ⁻¹)	Vapor Press. (atm)	Henry (atm L mol ⁻¹)	Kow [(mol L ⁻¹ octanol)/mol L ⁻¹ water]	Usage	Date of commercial availability
Chloromethane (<i>methyl chloride</i>)	CH ₃ Cl	$\begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{H} \\ \\ \text{Cl} \end{array}$	50.5	0.105	5.75	9.55	8.1	refrigerant; fumigant; synthesis	NA
Dichloromethane (<i>methylene chloride</i>)	CH ₂ Cl ₂	$\begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{Cl} \\ \\ \text{Cl} \end{array}$	84.9	0.230	0.589	2.57	14.1	solvent; dry-cleaner	NA
Trichloromethane (<i>chloroform</i>)	CHCl ₃	$\begin{array}{c} \text{Cl} \\ \\ \text{H}-\text{C}-\text{Cl} \\ \\ \text{Cl} \end{array}$	119.4	0.065	0.257	3.98	85.1	solvent; anesthetic; synthesis	1922
Tetrachloromethane (<i>carbon tetrachloride</i>)	CCl ₄	$\begin{array}{c} \text{Cl} \\ \\ \text{Cl}-\text{C}-\text{Cl} \\ \\ \text{Cl} \end{array}$	153.8	0.0063	0.154	24	537	solvent fumigant; dry-cleaner	1907
Trichlorofluoromethane (<i>Freon-11</i>)	CCl ₃ F	$\begin{array}{c} \text{Cl} \\ \\ \text{Cl}-\text{C}-\text{Cl} \\ \\ \text{F} \end{array}$	137.4	0.0083	1.05	126	145	refrigerant; aerosol propellant	NA
Trichloroethene	C ₂ HCl ₃	$\begin{array}{c} \text{Cl} \quad \quad \text{Cl} \\ \diagdown \quad \diagup \\ \text{C}=\text{C} \\ \diagup \quad \diagdown \\ \text{H} \quad \quad \text{Cl} \end{array}$	131.4	0.0091	0.098	10.7	263	solvent; dry-cleaner	1908
1,2-dibromoethane	C ₂ H ₂ Br ₂	$\begin{array}{c} \text{Br} \quad \text{Br} \\ \quad \\ \text{H}-\text{C}-\text{C}-\text{H} \\ \quad \\ \text{H} \quad \text{H} \end{array}$	187.9	0.0091	0.0027	0.295	91	gasoline additive; insecticide	NA

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Chlorinated pesticides

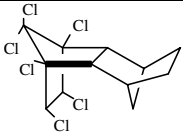
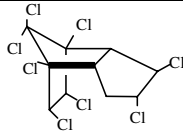
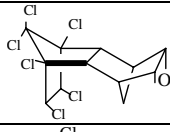
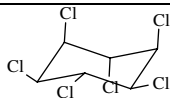
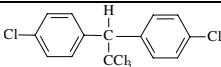
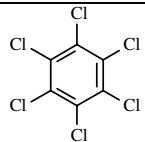
Compound name	Mol. Formula	Structure	Mol. Wgt.	Water Sol. (mol L ⁻¹)	Vapor Press. (atm)	Henry (atm L mol ⁻¹)	Kow [(mol L ⁻¹ octanol)/mol L ⁻¹ water]	Usage	Date of commercial availability
Aldrin	C ₁₂ H ₈ Cl ₆		362.9	4.6E-8	7.9E-9	0.17	330,000	pesticide	1948
Chlordane	C ₁₀ H ₆ Cl ₈		409.7	1.37E-7	1.28E-8	0.049	350,000	pesticide	1947
Dieldrin	C ₁₂ H ₈ Cl ₆ O		380.9	5.9E-7	2.1E-7	0.012	302,000	pesticide	1948
Lindane	C ₆ H ₆ Cl ₆		290.8	1.9E-4	6.3E-7	0.0032	6030	insecticide	NA
p,p'-DDT	C ₁₄ H ₉ Cl ₅		354.5	9.8E-8	9.3E-10	0.0095	2,300,000	pesticide	1942
Hexachlorobenzene	C ₆ Cl ₆		284.8	1.75E-8	2.43E-8	1.32	204,000	fungicide	~1940

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Aromatic hydrocarbons


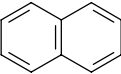
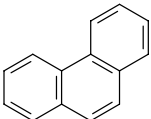
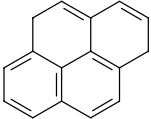
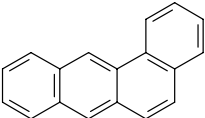
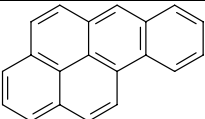
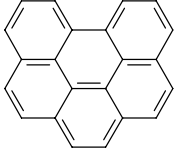
Compound name	Mol. Formula	Structure	Mol. Wgt.	Water Sol. (mol L ⁻¹)	Vapor Press. (atm)	Henry (atm L mol ⁻¹)	Kow [(mol L ⁻¹ octanol)/mol L ⁻¹ water]	Source
Benzene	C ₆ H ₆		78.1	0.23	0.13	5.5	135	solvent; fossil fuels; synthesis
Naphthalene	C ₁₀ H ₈		128.2	2.5E-4	3.7E-4	0.43	2300	fossil fuels; combustion of organic matter
Phenanthrene	C ₁₄ H ₁₀		178.2	6.3E-6	8.9E-7	0.026	37,000	fossil fuels; combustion of organic matter
Pyrene	C ₁₆ H ₁₀		202.3	6.7E-7	4.0E-8	0.0089	135,000	fossil fuels; combustion of organic matter
Benz(a)anthracene	C ₁₈ H ₁₂		228.3	4.9E-8	6.3E-9	0.0058	810,000	fossil fuels; combustion of organic matter
Benzo(a)pyrene	C ₂₀ H ₁₂		252.3	6.0E-9	2.3E-10	0.0012	3,200,000	fossil fuels; combustion of organic matter
Benzo(ghi)perylene	C ₂₂ H ₁₂		276.3	9.4E-10	1.3E-13	0.00015	3,800,000	fossil fuels; combustion of organic matter

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Additional industrial compounds

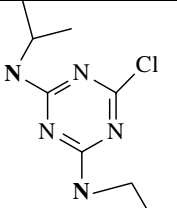
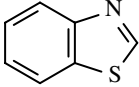
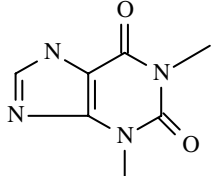
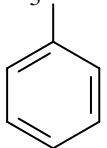
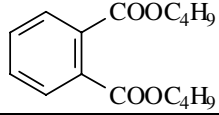
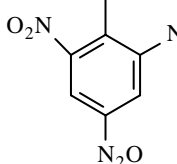
Compound name	Mol. Formula	Structure	Mol. Wgt.	Water Sol. (mol L ⁻¹)	Vapor Press. (atm)	Henry (atm L mol ⁻¹)	Kow [(mol L ⁻¹ octanol)/mol L ⁻¹ water)]	Usage	Date of commercial availability
Atrazine	C ₈ H ₁₄ ClN ₅		215.7	4.7E-3	3.8E-10	2.4E-6	360	herbicide	1959
Benzothiazole	C ₇ H ₅ NS		135.2	2.1E-2	1.4E-4	0.0065	100	breakdown product from rubber additive	-
Caffeine	C ₈ H ₁₀ N ₄ O ₂		194.2	0.11	-	1.9E-16	1	food and drink; additive	-
2-dodecylbenzene	C ₁₈ H ₃₀	CH ₃ CHC ₁₀ H ₂₃ 	246.4	4.5E-9	3.5E-7	-	1.5E8	detergent impurity	-
Di- <i>n</i> -butyl phthalate	C ₁₆ H ₂₂ O ₄		278.3	3.4E-5	9.5E-8	1.3E-3	37,000	plasticizer	~1940s
Trinitrotoluene	C ₇ H ₅ N ₃ O ₆		227.1	5.7E-4	1.1E-8	4.5E-4	40	explosive	~1905

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Chlorinated industrial compounds

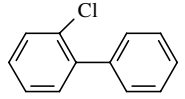
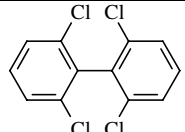
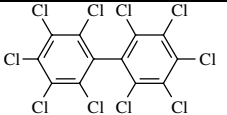
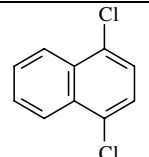
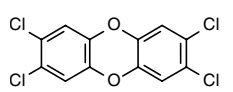
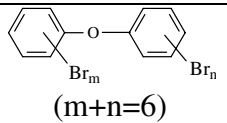
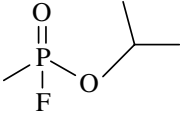
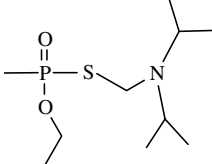
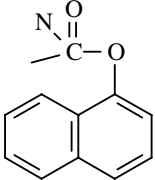
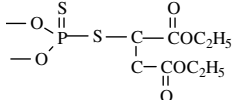
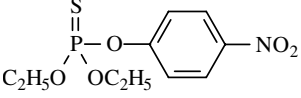
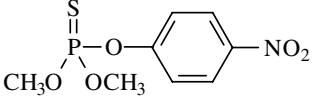
Compound name	Mol. Formula	Structure	Mol. Wgt.	Water Sol. (mol L ⁻¹)	Vapor Press. (atm)	Henry (atm L mol ⁻¹)	Kow [(mol L ⁻¹ octanol)/mol L ⁻¹ water]	Usage	Date of commercial availability
2-chlorobiphenyl	C ₁₂ H ₉ Cl		188.6	1.3E-4	2.5E-5	0.81	34,000	Mixtures used in electrical equipment	1929
2,2',5,5'-tetrachlorobiphenyl	C ₁₂ H ₆ Cl ₄		292.0	7.9E-7	2.3E-7	0.29	151,000	Mixtures used in electrical equipment	1929
decachlorobiphenyl	C ₁₂ Cl ₁₀		498.7	7.6E-9	1.4E-10	0.019	1.7E8	Mixtures used in electrical equipment	1929
1,4-dichloro naphthalene	C ₁₀ H ₆ Cl ₂		197.1	1.6E-6	2.3E-6	0.29	29,000	Mixtures used in electrical equipment	-
2,3,7,8-tetrachlorobenzo- <i>p</i> -dioxin	C ₁₂ H ₄ O ₂ Cl ₄		322.0	3.2E-8	1.6E-9	0.05	4,400,000	by-product of combustion	-
hexabromodiphenyl ether	C ₁₂ H ₂ Br ₆ O	 (m+n=6)	564.8	1.7E-12	-	-	6,800,000	flame retardant	~1960

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Organophosphates

Compound name	Mol. Formula	Structure	Mol. Wgt.	Water Sol. (mol L ⁻¹)	Vapor Press. (atm)	Henry (atm L mol ⁻¹)	Kow [(mol L ⁻¹ octanol)/mol L ⁻¹ water]	Usage	Date of commercial availability
Sarin (GB gas)	C ₄ H ₁₀ FO ₂ P		140.1	7.1	0.002	5.7E-4	6	chemical warfare agent	1938 (discovered)
VX gas	C ₁₁ H ₂₆ NO ₂ PS		267.4	0.1	9.2E-7	8.2E-6	115	chemical warfare agent	1952 (discovered)
carbaryl	C ₁₂ H ₁₁ NO ₂		201.2	5.5E-4	1.8E-9	3.3E-6	230	insecticide	1956
malathion	C ₁₀ H ₁₉ O ₆ PS ₂		330.4	4.3E-4	4.5E-9	4.9E-6	230	insecticide	1956
parathion	C ₁₀ H ₁₄ NO ₅ PS		291.3	3.8E-5	8.8E-9	3.0E-4	6770	insecticide	1947
methyl parathion	C ₈ H ₁₀ NO ₅ PS		263.2	1.4E-4	4.6E-9	1E-4	720	insecticide	1947