

Compounds subject to the Chemical Warfare Convention

TerraQSAR™ - LOGP computed octanol/water partition coefficients (CLOGPs).

For other toxicity and effect values, such as mammalian (rat/mouse) intravenous LD50, fish (fathead minnow) 96-hr LC50, estrogen receptor binding affinity (RBA), use TerraQSAR-RMIV, TerraQSAR-FHM, and TerraQSAR-E2-RBA programs, or consult TerraBase Inc.

SMILES	CAS	NAME	FORMULA	RTECS	MW	TerraQSAR-LOGP
<chem>N#CCl</chem>	506-77-4	chlorocyanide; cyanogen chloride	CCIN	GT 2275000	61.47	-0.18
<chem>O=C(Cl)Cl</chem>	75-44-5	phosgene	CCl2O	SY 5600000	98.92	1.16
<chem>O=N(=O)C(Cl)(Cl)Cl</chem>	76-06-2	chloropicrin; trichloronitromethane	CCl3NO2	PB 6300000	164.38	2.09
<chem>N#C</chem>	74-90-8	hydrogen cyanide	CHN	MW 6825000	27.03	-0.27
<chem>O=P(C)(Cl)Cl</chem>	676-97-1	methylphosphonyl dichloride	CH3Cl2OP	TA 1840000	132.91	1.00
<chem>O=P(F)(F)C</chem>	676-99-3	methylphosphonyl difluoride	CH3F2OP	TA 1840700	100	0.84
<chem>ClC=C[As](Cl)Cl</chem>	541-25-3	2-chlorovinyl dichloroarsine; Lewisite	C2H2AsCl3	CH 2975000	207.32	2.08
<chem>O=P([H])(OC)OC</chem>	868-85-9	dimethyl phosphite	C2H7O3P	SZ 7710000	110.05	-0.65
<chem>C(Cl)CSC(Cl)</chem>	2625-76-5	2-chloroethyl chloromethyl sulfide	C3H6Cl2S	-	145.05	1.17
<chem>O(P(OC)OC)C</chem>	121-45-9	trimethyl phosphite; phosphorous acid, trimethyl ester	C3H9O3P	TH 1400000	124.08	-0.18
<chem>O=P(OC)(OC)C</chem>	756-79-6	dimethylmethylphosphonate	C3H9O3P	SZ 9120000	124.08	-0.55
<chem>FC(F)=C(C(F)(F)F)C(F)(F)F</chem>	382-21-8	octafluoroisobutene	C4F8	UD 1800000	200.03	1.71
<chem>C(Cl)=C[As](Cl)C=C(Cl)</chem>	40334-69-8	bis(2-chlorovinyl)chloroarsine; Lewisite 2	C4H4AsCl3	CG 8350000	233.36	2.28
<chem>C1CCSCCC1</chem>	505-60-2	bis(2-chloroethyl) sulfide; Sulfur Mustard	C4H8Cl2S	WQ 0900000	159.07	1.25
<chem>O=P(Cl)(C)OC(C)C</chem>	1445-76-7	Chlorosarin; phosphonochloridic acid, methyl-, 1-methylethyl ester	C4H10ClO2P	-	156.55	0.30
<chem>O=P(F)(C)OC(C)C</chem>	107-44-8	Sarin; O-isopropylmethylphosphonofluoridate; phosphonofluoridic acid, methyl-, 1-methylethyl ester	C4H10FO2P	TA 8400000	140.09	0.46
<chem>OCCSCCO</chem>	111-48-8	bis(2-hydroxyethyl)sulfide	C4H10O2S	KM 2975000	122.18	-0.57
<chem>OCCN(C)C</chem>	108-01-0	N,N-dimethylaminoethanol; deanol	C4H11NO	KK 6125000	89.14	0.18
<chem>O=P([H])(OCC)OCC</chem>	762-04-9	phosphonic acid, diethyl ester; diethyl phosphite	C4H11O3P	TG 7875000	138.1	0.74
<chem>C1CCSCSCC1</chem>	63869-13-6	bis(2-chloroethylthio)methane	C5H10Cl2S2	-	205.16	0.77
<chem>CN(CCCl)CCCl</chem>	51-75-2	bis(2-chloroethyl)methylamine; Mechlorethamine; HN2	C5H11Cl2N	IA 1750000	156.05	1.08

<chem>O=P(C#N)(OCC)N(C)C</chem>	77-81-6	Tabun; O-ethyl N,N-dimethylphosphoramidocyanidate; phosphoramidocyanidic acid, dimethyl-, ethyl ester	C5H11N2O2P	TB 4550000	162.13	0.38
<chem>O=P(F)(CC)OC(C)C</chem>	1189-87-3	GE; phosphonofluoridic acid, ethyl-, isopropyl ester	C5H12FO2P	TA 8110000	154.12	0.30
<chem>OCCN(CCO)C</chem>	105-59-9	N-methyldiethanolamine	C5H13NO2	KL 7525000	119.16	-1.02
<chem>CIC=C[As](C=C(Cl))C=C(Cl)</chem>	40334-70-1	tris(2-chlorovinyl)arsine	C6H6AsCl3	-	259.39	2.74
<chem>CICCSCOCSCCCI</chem>	63918-90-1	bis(2-chloroethylthiomethyl)ether	C6H12Cl2OS2	-	235.19	0.77
<chem>CICCSCCSCCCI</chem>	3563-36-8	1,2-bis(2-chloroethylthio)ethane	C6H12Cl2S2	KH 5425000	219.19	0.77
<chem>CICCN(CCCI)CCCI</chem>	555-77-1	tris(2-chloroethyl)amine	C6H12Cl3N	YE 2625000	204.53	0.91
<chem>CCN(CCCI)CCCI</chem>	538-07-8	bis(2-chloroethyl)ethylamine	C6H13Cl2N	YE 1225000	170.08	0.91
<chem>OC(C(C)(C)C)C</chem>	464-07-3	3,3-dimethylbutan-2-ol; pinacolyl alcohol	C6H14O	EL 2276000	102.18	1.48
<chem>OCCN(CC)CC</chem>	100-37-8	N,N-diethylethanolamine	C6H15NO	KK 5075000	117.19	0.92
<chem>OCCN(CCO)CC</chem>	139-87-7	N-ethyldiethanolamine	C6H15NO2	KK 9800000	133.19	-0.82
<chem>OCCN(CCO)CCO</chem>	102-71-6	triethanolamine	C6H15NO3	KL 9275000	149.19	-1.00
<chem>P(OCC)(OCC)OCC</chem>	122-52-1	triethyl phosphite; phosphorous acid, triethyl ester	C6H15O3P	TH 1130000	166.16	0.93
<chem>OC(C(CCN1C2)C2)C1</chem>	1619-34-7	quinuclidine-3-ol; 1-azabicyclo[2.2.2]octan-3-ol	C7H13NO	VD 6191700	127.19	1.35
<chem>CICCSCCCSCCCI</chem>	63905-10-2	1,3-bis(2-chloroethylthio)-n-propane	C7H14Cl2S2	-	233.21	0.77
<chem>O=P(Cl)(C)OC(C)C(C)C(C)C</chem>	7040-57-5	Chlorosoman; phosphonochloridic acid, methyl-, 1,2,2-trimethylpropyl ester	C7H16ClO2P	TA 3650000	198.63	1.78
<chem>CC(OP(C)(F)=O)C(C)(C)C</chem>	96-64-0	Soman; O-pinacolyl methylphosphonofluoridate; phosphonofluoridic acid, methyl-, 1,2,2-trimethylpropyl ester	C7H16FO2P	TA 8750000	182.17	1.78
<chem>CICCSCCOCSCCCI</chem>	63918-89-8	bis(2-chloroethylthioethyl)ether; Agent T	C8H16Cl2OS2	KN 1400000	263.24	0.77
<chem>CICCSCCCSCCCI</chem>	142868-93-7	1,4-bis(2-chloroethylthio)-n-butane	C8H16Cl2S2	-	247.24	0.77
<chem>CICCSCCCSCCCI</chem>	142868-94-8	1,5-bis(2-chloroethylthio)-n-pentane	C9H18Cl2S2	-	261.27	0.77
<chem>OC1(O)CCN2C(=N)\N[C@@]([H])(COC(=O)N)[C@@]3([H])N(C(=N)N[C@@]12)3</chem>	35523-89-8	saxitoxin; 1H,10H-pyrrolo[1,2-c]purine-10,10-diol, 2,6-diamino-4-[[[(aminocarbonyloxy)methyl]-3a,4,8,9-tetrahydro-, (3aS,4R,10aS)-	C10H17N7O4	UY 8708500	299.29	-0.85
<chem>O=P(SCCN(CC)CC)(OCC)OCC</chem>	78-53-5	Amiton; phosphorothioic acid, S-[2-(diethylamino)ethyl] O,O-diethyl ester	C10H24NO3PS	TF 0525000	269.34	-0.68

<chem>O=P(C)(OCC)SCCN(C(C)C)C(C)C</chem>	50782-69-9	VX; O-ethyl S-2-diisopropylaminoethyl methyl phosphonodithioate; phosphonothioic acid, methyl-, S-[2-[bis(1-methylethyl)amino]ethyl] O-ethyl ester	C11H26NO2PS	TB 1090000	267.37	2.09
<chem>O=P(C)(OCC)OCCN(C(C)C)C(C)C</chem>	57856-11-8	O-ethyl O-2-diisopropylaminoethylmethylphosphonite; phosphonous acid, methyl-, 2-[bis(1-methylethyl)amino]ethyl ethyl ester	C11H26NO3P	-	251.31	1.01
<chem>O=C(O)C(O)(c(cccc1)c1)c(cccc2)c2</chem>	76-93-7	2,2-diphenyl-2-hydroxyacetic acid; benzilic acid	C14H12O3	DD 2064000	228.25	2.30
<chem>N12CCC(CC1)C(OC(=O)C(O)(c1ccccc1)c1ccc1)C2</chem>	6581-06-2	3-quinuclidinyl benzilate; BZ; benzeneacetic acid, .alpha.-hydroxy-.alpha.-phenyl-, 1-azabicyclo[2.2.2]oct-3-yl ester	C21H23NO3	DD 4638000	337.42	4.70
<chem>[As](Cl)(Cl)Cl</chem>	7784-34-1	arsenic trichloride	AsCl3	CG 1750000	181.28	
<chem>O=S(Cl)Cl</chem>	7719-09-7	thionyl chloride	Cl2OS	XM 5150000	118.97	
<chem>ClSCl</chem>	10545-99-0	sulfur dichloride	Cl2S	-	102.97	
<chem>ClSSCl</chem>	10025-67-9	disulfur dichloride (S2Cl2)	Cl2S2	WS 4300000	135.03	
<chem>ClP(Cl)(Cl)=O</chem>	10025-87-3	phosphorus oxide trichloride	Cl3OP	TH 8970000	153.33	
<chem>ClP(Cl)Cl</chem>	7719-12-2	phosphorus trichloride	Cl3P	TH 3675000	137.33	
<chem>ClP(Cl)(Cl)(Cl)Cl</chem>	10026-13-8	phosphorus pentachloride	Cl5P	TB 6125000	208.24	

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