Mirex

Other names:	1,1a,2,2,3,3a,4,5,5,5a,5b,6-Dodecachlorooctahydro-1,3,4-metheno-1H-cyclobuta(cd)pent
	1,2,3,4,5,5-Hexachloro-1,3-cyclopentadiene dimer
	1,3,4-Metheno-1H-cyclobuta(cd)pentalene, dodecachlorooctahydro-
	1,3,4-Metheno-1H-cyclobuta[cd]pentalene, 1,1a,2,2,3,3a,4,5,5,5a,5b,6-dodecachlorooctahydro-
	1,3,4-Metheno-2H-cyclobuta[cd]pentalene, dodecachlorooctahydro-
	1,3-Cyclopentadiene, 1,2,3,4,5,5-hexachloro-, dimer
	2385-85-5
	Bichlorendo
	CG-1283
	Cyclopentadiene, hexachloro-, dimer
	Decane,perchloropentacyclo-
	Dechlorane
	Dechlorane 4070
	Dodecachlorooctahydro-1,3,4-metheno-1H-cyclobuta(cd)pentalene
	Dodecachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalene
	Dodecachloropentacyclo(3,3,2,0(2,6),0(3,9),0(7,10))decane
	Dodecachloropentacyclodecane
	ENT 25,719
	Ferriamicide
	GC 1283
	HRS l276
	Hexachlorocyclopentadiene Dimer
	NCI-C06428
	NSC 26107
	NSC 37656
	Paramex
	Pentacyclodecane, dodecachloro-
	Perchlorodihomocubane
	Perchloropentacyclo(5.2.1.0(2,6),0(3,9),0(5,8)decane
	Perchloropentacyclo[5.2.1.0(2,6).0(3,9).0(5,8)]decane
	Perchloropentacyclodecane
	dodecachloropentacyclo[5.2.1.02,6.03,9.05,8]decane
Inchi:	InChI=1S/C10Cl12/c11-1-2(12)7(17)4(14)3(13,5(1,15)9(7,19)20)6(1,16)10(21,22)8(2,4)18
InchiKey:	GVYLCNUFSHDAAW-UHFFFAOYSA-N
Formula:	C10Cl12
SMILES:	ClC1(Cl)C2(Cl)C3(Cl)C4(Cl)C(Cl)(Cl)C5(Cl)C3(Cl)C1(Cl)C5(Cl)C24Cl
Mol. weight [g/mol]:	545.54
CAS:	2385-85-5

Physical Properties

Property code	Value	Unit	Source
gf	160.96	kJ/mol	Joback Method
hf	6.89	kJ/mol	Joback Method
hfus	15.57	kJ/mol	Joback Method
hvap	76.12	kJ/mol	Joback Method
log10ws	-6.80		Aqueous Solubility Prediction Method
log10ws	-6.80		Estimated Solubility Method
logp	6.223		Crippen Method
mcvol	244.340	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	2494.00		NIST Webbook
rinpol	2470.00		NIST Webbook
rinpol	2470.00		NIST Webbook
rinpol	2470.00		NIST Webbook
rinpol	2472.00		NIST Webbook
ripol	3348.00		NIST Webbook
ripol	3348.00		NIST Webbook
tb	868.76	K	Joback Method
tc	1210.15	K	Joback Method
tf	886.60	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.66	J/mol×K	1153.25	Joback Method
cpg	502.59	J/mol×K	868.76	Joback Method
cpg	544.69	J/mol×K	925.66	Joback Method
cpg	607.06	J/mol×K	982.56	Joback Method
cpg	693.78	J/mol×K	1039.45	Joback Method
cpg	808.95	J/mol×K	1096.35	Joback Method
cpg	1140.99	J/mol×K	1210.15	Joback Method
hvapt	90.30	kJ/mol	398.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2385855&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume