Kepone

Other names:	1,1a,3,3a,4,5,5,5a,5b,6-Decachlorooctahydro-1,3,4-metheno-2H-cyclobuta(cd)pentalen-2
	1,2,3,5,6,7,8,9,10,10-Decachloro(5.2.1.0(2,6).0(3,9) .0(5,8))decan-4-one
	1,3,4-Metheno-2H-cyclobuta(cd)pentalen-2-one, 1,1a,3,3a,4,5,5,5a,5b,6-decachlorooctahydro-
	1,3,4-Metheno-2H-cyclobuta[cd]pentalen-2-one, 1,1a,3,3a,4,5,5,5a,5b,6-decachlorooctahydro-
	143-50-0
	Chlordecone
	Chlorodecone
	Ciba 8514
	Clordecone
	Compound 1189
	Decachloro-1,3,4-metheno-2H-cyclobuta(cd)pentalen-2-one
	Decachloroketone
	Decachlorooctahydro-1,3,4-metheno-2H-cyclobuta(cd)pentalen-2-one
	Decachlorooctahydro-1,3,4-metheno-2H-cyclobuta[cd]pentalin-2-one
	Decachloropentacyclo(5.3.0.0(2,6).0(4,10).0(5,9))decan-3-one
	Decachloropentacyclo[5.2.1.0(2,6).0(3,9).0(5,8)]decan-4-one
	Decachlorotetracyclodecanone
	Decachlorpentacyclo (5.2.1.0(2,6).0(3,9).0(5,8)) decan-4-one
	ENT 16,391
	ENT-16391
	GC 1189
	General chemicals 1189
	Kepone-2-one, decachlorooctahydro-
	Merex
	NCI-C00191
	NSC 124074
	Rcra waste number U142
Inchi:	InChI=1S/C10Cl10O/c11-2-1(21)3(12)6(15)4(2,13)8(17)5(2,14)7(3,16)9(6,18)10(8,19)20
InchiKey:	LHHGDZSESBACKH-UHFFFAOYSA-N
Formula:	C10Cl10O
SMILES:	O=C1C2(Cl)C3(Cl)C4(Cl)C(Cl)(Cl)C5(Cl)C3(Cl)C1(Cl)C5(Cl)C24Cl
Mol. weight [g/mol]:	490.64
CAS:	143-50-0

Physical Properties

Property code	Value	Unit	Source

gf	75.43	kJ/mol	Joback Method
hf	-94.23	kJ/mol	Joback Method
hfus	11.91	kJ/mol	Joback Method
hvap	73.06	kJ/mol	Joback Method
log10ws	-5.26		Estimated Solubility Method
log10ws	-5.26		Aqueous Solubility Prediction Method
logp	4.618		Crippen Method
mcvol	221.430	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
rinpol	2222.00		NIST Webbook
rinpol	2222.00		NIST Webbook
rinpol	2222.00		NIST Webbook
rinpol	2240.00		NIST Webbook
tb	866.15	K	Joback Method
tc	1203.16	K	Joback Method
tf	875.32	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.58	J/mol×K	866.15	Joback Method
cpg	517.60	J/mol×K	922.32	Joback Method
cpg	572.94	J/mol×K	978.49	Joback Method
cpg	649.12	J/mol×K	1034.65	Joback Method
cpg	749.65	J/mol×K	1090.82	Joback Method
cpg	878.02	J/mol×K	1146.99	Joback Method
cpg	1037.76	J/mol×K	1203.16	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C143500&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume