o,p'-DDE

Other names:	1,1-Dichloro-2-(o-chlorophenyl)-2-(p-chlorophenyl)ethene 1,1-Dichloro-2-(o-chlorophenyl)-2-(p-chlorophenyl)ethylene 1-Chloro-2-(2,2-dichloro-1-(4-chlorophenylethenyl)benzene 1-chloro-4-[2,2-dichloro-1-(2-chlorophenyl)ethenyl]benzene 2,2,o,p'-tetrachlorovinylidenebisbenzene 2,4'-DDE 2-(2-Chlorophenyl)-2-(4-chlorophenyl)-1,1-dichloroethylene Benzene, 1-chloro-2-[2,2-dichloro-1-(4-chlorophenyl)ethenyl]- Ethylene, 1,1-dichloro-2-(o-chlorophenyl)-2-(p-chlorophenyl)- Ethylene, 1-(o-chlorophenyl)-1-(p-chlorophenyl)-2,2-dichloro- NSC 59908 o,p-DDE
Inchi:	InChI=1S/C14H8Cl4/c15-10-7-5-9(6-8-10)13(14(17)18)11-3-1-2-4-12(11)16/h1-8H
InchiKey:	ZDYJWDIWLRZXDB-UHFFFAOYSA-N
Formula:	C14H8Cl4
SMILES:	ClC(Cl)=C(c1ccc(Cl)cc1)c1ccccc1Cl
Mol. weight [g/mol]:	318.02
CAS:	3424-82-6

Physical Properties

Property code	Value	Unit	Source
gf	287.96	kJ/mol	Joback Method
hf	152.51	kJ/mol	Joback Method
hfus	33.69	kJ/mol	Joback Method
hvap	70.29	kJ/mol	Joback Method
log10ws	-6.36		Aqueous Solubility Prediction Method
logp	6.188		Crippen Method
mcvol	205.260	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
rinpol	2054.00		NIST Webbook
rinpol	2057.00		NIST Webbook
rinpol	2047.00		NIST Webbook
rinpol	2053.00		NIST Webbook
rinpol	2072.00		NIST Webbook
rinpol	2072.00		NIST Webbook
rinpol	2070.00		NIST Webbook

rinpol	2050.00		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	2055.00		NIST Webbook
rinpol	2054.00		NIST Webbook
rinpol	2051.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2046.00		NIST Webbook
rinpol	2046.00		NIST Webbook
ripol	2904.00		NIST Webbook
ripol	2895.00		NIST Webbook
tb	736.68	K	Joback Method
tc	1008.88	K	Joback Method
tf	351.54 ± 0.20	K	NIST Webbook
tf	351.40 ± 0.20	K	NIST Webbook
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.87	J/mol×K	736.68	Joback Method
cpg	457.47	J/mol×K	782.05	Joback Method
cpg	467.99	J/mol×K	827.41	Joback Method
cpg	477.54	J/mol×K	872.78	Joback Method
cpg	486.29	J/mol×K	918.15	Joback Method
cpg	494.35	J/mol×K	963.52	Joback Method
cpg	501.87	J/mol×K	1008.88	Joback Method
hfust	23.84	kJ/mol	349.80	NIST Webbook

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3424826&Units=SI

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
hfust:	Enthalpy of fusion at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume