p,p'-DDE

Other names:	1,1'-(Dichloroethenylidene)bis(4-chlorobenzene) 1,1-Bis(p-chlorophenyl)-2,2-dichloroethylene 1,1-Dichloro-2,2-Bis(p-chlorophenyl)ethylene 1,1-Dichloro-2,2-bis(4-chlorophenyl)ethylene (p,p'-DDE) 1,1-Dichloro-2,2-bis(p-chlorophenyl)ethene 1,1-Dichloro-2,2-di(p-chlorophenyl)ethylene 1-chloro-4-[2,2-dichloro-1-(4-chlorophenyl)ethenyl]benzene 2,2-Bis(4-chlorophenyl)-1,1-dichloroethene 2,2-Bis(4-chlorophenyl)-1,1-dichloroethylene 2,2-Bis(p-chlorophenyl)-1,1-dichloroethylene 4,4'-DDE Benzene, 1,1'-(dichloroethenylidene)bis[4-chloro- DDE DDE(p,p') DDT dehydrochloride Dichlorodiphenyldichloroethylene Ethylene, 1,1-dichloro-2,2-bis(p-chlorophenyl)- NCI-C00555 NSC 1153 p,p'-(Dichlorodiphenyl)-2,2-dichloroethylene p,p'-Dichlorodiphenyldichloroethylene p,p-Dde
Inchi:	InChI=1S/C14H8Cl4/c15-11-5-1-9(2-6-11)13(14(17)18)10-3-7-12(16)8-4-10/h1-8H
InchiKey:	UCNVFOCBFJOQAL-UHFFFAOYSA-N
Formula:	C14H8Cl4
SMILES:	ClC(Cl)=C(c1ccc(Cl)cc1)c1ccc(Cl)cc1
Mol. weight [g/mol]:	318.02
CAS:	72-55-9

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	-6.90		Estimated Solubility Method

log10ws	-6.90		Aqueous Solubility Prediction Method
logp	6.188		Crippen Method
mcvol	205.260	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
rinpol	2180.00		NIST Webbook
rinpol	2116.00		NIST Webbook
rinpol	2111.00		NIST Webbook
rinpol	2120.00		NIST Webbook
rinpol	2113.00		NIST Webbook
rinpol	2117.00		NIST Webbook
rinpol	2116.00		NIST Webbook
rinpol	2121.00		NIST Webbook
rinpol	2112.00		NIST Webbook
rinpol	2208.00		NIST Webbook
rinpol	2196.00		NIST Webbook
rinpol	2192.00		NIST Webbook
rinpol	2113.00		NIST Webbook
rinpol	2110.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	362.90		NIST Webbook
rinpol	2196.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2113.00		NIST Webbook
rinpol	2117.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2136.00		NIST Webbook
rinpol	2132.00		NIST Webbook
rinpol	2111.00		NIST Webbook
rinpol	2208.00		NIST Webbook
ripol	2990.00		NIST Webbook
tb	736.68	K	Joback Method
tc	1008.88	K	Joback Method
tf	360.56 ± 0.20	K	NIST Webbook
tf	363.00 ± 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	23.55	kJ/mol	360.40	NIST Webbook
hvapt	87.20	kJ/mol	398.00	NIST Webbook

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=C72559&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
hfust: Enthalpy of fusion at a given temperature
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