Benzene, 1-chloro-2-[2,2-dichloro-1-(4-chlorophenyl)etheny

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
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]: 318.03

Physical Properties

Property code	Value	Unit	Source
hf	166.94	kJ/mol	Cheméo Relay (1.0)
hfus	33.69	kJ/mol	Joback Method
ie	8.19	eV	Cheméo Relay (1.0)
log10ws	-6.36		Aqueous Solubility Prediction Method
logp	6.188		Crippen Method
mcvol	205.260	ml/mol	McGowan Method
tb	620.11	K	Cheméo Relay (1.0)
tf	344.00	K	Cheméo Relay (1.0)

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

Sources

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point