o,p'-DDT

Other names: (.+/-.)-1-(o-Chlorophenyl)-1-(p-chlorophenyl)-2,2,2-trichloroethane
1,1,1-Trichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane
1,1,1-Trichloro-2-(4-chlorophenyl)-2-(2-chlorophenyl)ethane (p,o'-DDT)
1,1,1-Trichloro-2-(o-chlorophenyl)-2-(p-chlorophenyl)ethane
1-(o-Chlorophenyl)-1-(p-chlorophenyl)-2,2,2-trichloro ethane
1-Chloro-2-[2,2,2-trichloro-1-(4-chlorophenyl)ethyl]benzene
1-chloro-4-[2,2,2-trichloro-1-(2-chlorophenyl)ethyl]benzene
2,2,2,o,p'-pentachloroethylidenebisbenzene
2,2-Bis(o,p-chlorophenyl)-1,1,1-trichloroethane
2,4'-DDT
2-(2-Chlorophenyl)-2-(4-chlorophenyl)-1,1,1-trichloroethane
Benzene, 1-chloro-2-[2,2,2-trichloro-1-(4-chlorophenyl)ethyl]-
DDT-o,p'
Ethane, 1,1,1-trichloro-2-(o-chlorophenyl)-2-(p-chlorophenyl)-
Ethane, 2-(o-chlorophenyl)-2-(p-chlorophenyl)-1,1,1-trichloro-
NSC 33446
NSC 57644
o,p-DDT

Inchi: InChI=1S/C14H9Cl5/c15-10-7-5-9(6-8-10)13(14(17,18)19)11-3-1-2-4-12(11)16/h1-8,13H

InchiKey: CVUGPAFCQJIYDT-UHFFFAOYSA-N

Formula: C14H9Cl5

SMILES: Clc1ccc(C(c2ccccc2Cl)C(Cl)(Cl)Cl)cc1

Mol. weight [g/mol]: 354.49

CAS: 789-02-6

Physical Properties

Property code	Value	Unit	Source
gf	213.31	kJ/mol	Joback Method
hf	25.10	kJ/mol	Joback Method
hfus	29.37	kJ/mol	Joback Method
hvap	72.88	kJ/mol	Joback Method
log10ws	-6.62		Aqueous Solubility Prediction Method
logp	6.495		Crippen Method
mcvol	221.800	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
rinpol	2220.00		NIST Webbook

rinpol	2199.00		NIST Webbook
ripol	3127.00		NIST Webbook
tb	766.52	K	Joback Method
tc	1041.34	K	Joback Method
tf	349.00 ± 0.20	K	NIST Webbook
tf	347.75	K	Aqueous Solubility Prediction Method
tf	346.97 ± 0.20	K	NIST Webbook
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.29	J/mol×K	766.52	Joback Method
cpg	506.48	J/mol×K	812.32	Joback Method
cpg	516.50	J/mol×K	858.13	Joback Method
cpg	525.51	J/mol×K	903.93	Joback Method
cpg	533.67	J/mol×K	949.73	Joback Method
cpg	541.13	J/mol×K	995.53	Joback Method
cpg	548.06	J/mol×K	1041.34	Joback Method
dvisc	0.0005214	Pa×s	513.12	Joback Method
dvisc	0.0009338	Pa×s	462.44	Joback Method
dvisc	0.0003233	Pa×s	563.80	Joback Method
dvisc	0.0002169	Pa×s	614.48	Joback Method
dvisc	0.0001547	Pa×s	665.16	Joback Method
dvisc	0.0001157	Pa×s	715.84	Joback Method
dvisc	0.0000899	Pa×s	766.52	Joback Method
hfust	23.09	kJ/mol	345.80	NIST Webbook
hvapt	88.60	kJ/mol	398.00	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=C789026&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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