1,1-Dichloro-2,2-bis(p-chlorophenyl)ethane

Other names:
1,1-Bis(4-chlorophenyl)-2,2-dichloroethane
1,1-Bis(p-Chlorophenyl)-2,2-dichloroethane
1,1-Dichloor-2,2-bis(4-chloor fenyl)-ethaan
1,1-Dichlor-2,2-bis(4-chlor-phenyl)-aethan
1,1-Dichloro-2,2-bis(4-chlorophenyl)ethane
1,1-Dichloro-2,2-bis(4-chlorophenyl)ethane p,p'-DDD
1,1-Dichloro-2,2-bis(parachlorophenyl)ethane
1,1-Dichloro-2,2-di(4-chlorophenyl)ethane
1,1-Dicloro-2,2-bis(4-cloro-fenil)-etano
1-chloro-4-[2,2-dichloro-1-(4-chlorophenyl)ethyl]benzene
2,2-Bis(4-chlorophenyl)-1,1-dichloroethane
2,2-Bis(p-chlorophenyl)-1,1-dichloroethane
4,4'-DDD
Benzene, 1,1'-(2,2-dichloroethylidene)bis[4-chloro-
DDD
DDD(p,p')
Dichlorodiphenyldichloroethane
Dilene
ENT 4,225
Ethane, 1,1-dichloro-2,2-bis(4-chlorophenyl)-
Ethane, 1,1-dichloro-2,2-bis(p-chlorophenyl)-
ME1700
NCI-C00475
NSC 8941
OMS 1078
Rcra waste number U060
Rhothane
Rhothane D-3
Rothane
TDE
Tetrachlorodiphenylethane
p,p'-(Dichlorodiphenyl)dichloroethane
p,p'-DDD
p,p'-Dichlorodiphenyl-2,2-dichloroethylene
p,p'-TDE
p,p-Ddd

Inchi: InChI=1S/C14H10Cl4/c15-11-5-1-9(2-6-11)13(14(17)18)10-3-7-12(16)8-4-10/h1-8,13-14H

InchiKey: AHJKRLASYNVKDZ-UHFFFAOYSA-N

Formula: C14H10Cl4

SMILES: Clc1ccc(C(c2ccc(Cl)cc2)C(Cl)Cl)cc1

Mol. weight [g/mol]: 320.04
CAS: 72-54-8

Physical Properties

Property code	Value	Unit	Source
gf	219.96	kJ/mol	Joback Method
hf	44.31	kJ/mol	Joback Method
hfus	29.06	kJ/mol	Joback Method
hvap	69.40	kJ/mol	Joback Method
log10ws	-7.20		Aqueous Solubility Prediction Method
log10ws	-7.20		Estimated Solubility Method
logp	5.929		Crippen Method
mcvol	209.560	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	2208.00		NIST Webbook
rinpol	2203.00		NIST Webbook
rinpol	2203.00		NIST Webbook
rinpol	2213.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2212.00		NIST Webbook
rinpol	2196.00		NIST Webbook
rinpol	2272.00		NIST Webbook
rinpol	2213.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2196.00		NIST Webbook
rinpol	2199.00		NIST Webbook
rinpol	2272.00		NIST Webbook
rinpol	2208.00		NIST Webbook
rinpol	2200.00		NIST Webbook
ripol	3310.00		NIST Webbook
tb	731.88	K	Joback Method
tc	994.89	K	Joback Method
tf	382.30 ± 0.20	K	NIST Webbook
tf	382.40	K	Aqueous Solubility Prediction Method
tf	383.41 ± 0.20	K	NIST Webbook
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.22	J/mol×K	951.06	Joback Method
cpg	531.79	J/mol×K	994.89	Joback Method
cpg	472.46	J/mol×K	731.88	Joback Method
cpg	484.99	J/mol×K	775.72	Joback Method
cpg	496.33	J/mol×K	819.55	Joback Method
cpg	506.59	J/mol×K	863.39	Joback Method
cpg	515.85	J/mol×K	907.22	Joback Method
dvisc	0.0001154	Pa×s	731.88	Joback Method
dvisc	0.0001482	Pa×s	679.08	Joback Method
dvisc	0.0013431	Pa×s	415.10	Joback Method
dvisc	0.0007083	Pa×s	467.90	Joback Method
dvisc	0.0004253	Pa×s	520.69	Joback Method
dvisc	0.0002805	Pa×s	573.49	Joback Method
dvisc	0.0001984	Pa×s	626.29	Joback Method
hfust	27.31	kJ/mol	382.10	NIST Webbook
hvapt	88.50	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=C72548&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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