

2,2',3,3',4',5,6-Heptachlorodiphenyl ether

Inchi:	InChI=1S/C12H3Cl7O/c13-4-1-2-7(11(19)8(4)16)20-12-9(17)5(14)3-6(15)10(12)18/h1-3H
InchiKey:	RXPQVFMDOJTCKE-UHFFFAOYSA-N
Formula:	C12H3Cl7O
SMILES:	Clc1ccc(Oc2c(Cl)c(Cl)cc(Cl)c2Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	411.33

Physical Properties

Property code	Value	Unit	Source
gf	19.06	kJ/mol	Joback Method
hf	-140.64	kJ/mol	Joback Method
hfus	42.76	kJ/mol	Joback Method
hvap	84.60	kJ/mol	Joback Method
log10ws	-9.09		Aqueous Solubility Prediction Method
logp	8.053		Crippen Method
mcvol	223.970	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
tb	846.61	K	Joback Method
tc	1114.35	K	Joback Method
tf	597.15	K	Joback Method
vc	0.853	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.95	J/molxK	846.61	Joback Method
cpg	443.65	J/molxK	891.23	Joback Method
cpg	449.51	J/molxK	935.86	Joback Method
cpg	454.54	J/molxK	980.48	Joback Method
cpg	458.75	J/molxK	1025.10	Joback Method
cpg	462.15	J/molxK	1069.73	Joback Method
cpg	464.76	J/molxK	1114.35	Joback Method
dvisc	0.0003259	Paxs	597.15	Joback Method
dvisc	0.0002490	Paxs	638.73	Joback Method

dvisc	0.0001966	Paxs	680.30	Joback Method
dvisc	0.0001595	Paxs	721.88	Joback Method
dvisc	0.0001324	Paxs	763.46	Joback Method
dvisc	0.0001120	Paxs	805.03	Joback Method
dvisc	0.0000964	Paxs	846.61	Joback Method

Sources

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

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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