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

Inchi: InChI=1S/C12H3Cl7O/c13-5-2-1-4(3-6(5)14)20-12-10(18)8(16)7(15)9(17)11(12)19/h1-3H

InchiKey: QLSBRXLSQINWHM-UHFFFAOYSA-N

Formula: C12H3Cl7O

SMILES: Clc1ccc(Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)cc1Cl

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	-9.46		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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.95	J/mol×K	846.61	Joback Method
cpg	462.15	J/mol×K	1069.73	Joback Method
cpg	458.75	J/mol×K	1025.10	Joback Method
cpg	454.54	J/mol×K	980.48	Joback Method
cpg	449.51	J/mol×K	935.86	Joback Method
cpg	443.65	J/mol×K	891.23	Joback Method
cpg	464.76	J/mol×K	1114.35	Joback Method
dvisc	0.0000964	Pa×s	846.61	Joback Method
dvisc	0.0001120	Pa×s	805.03	Joback Method

dvisc	0.0001324	Pa×s	763.46	Joback Method
dvisc	0.0001595	Pa×s	721.88	Joback Method
dvisc	0.0001966	Pa×s	680.30	Joback Method
dvisc	0.0002490	Pa×s	638.73	Joback Method
dvisc	0.0003259	Pa×s	597.15	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/ci990307l
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