Decachlorodiphenyl ether

Inchi: InChI=1S/C12Cl10O/c13-1-3(15)7(19)11(8(20)4(1)16)23-12-9(21)5(17)2(14)6(18)10(12)2
InchiKey: CIPFDHFTBYJKQB-UHFFFAOYSA-N
Formula: C12Cl10O
SMILES: Clc1c(Cl)c(Cl)c(Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 514.66

Physical Properties

Property code	Value	Unit	Source
gf	-45.62	kJ/mol	Joback Method
hf	-222.27	kJ/mol	Joback Method
hfus	54.19	kJ/mol	Joback Method
hvap	99.74	kJ/mol	Joback Method
log10ws	-12.95		Aqueous Solubility Prediction Method
logp	10.013		Crippen Method
mcvol	260.690	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
tb	973.84	K	Joback Method
tc	1246.84	K	Joback Method
tf	724.47	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.09	J/mol×K	973.84	Joback Method
cpg	478.44	J/mol×K	1201.34	Joback Method
cpg	478.57	J/mol×K	1155.84	Joback Method
cpg	477.79	J/mol×K	1110.34	Joback Method
cpg	476.10	J/mol×K	1064.84	Joback Method
cpg	473.53	J/mol×K	1019.34	Joback Method
cpg	477.37	J/mol×K	1246.84	Joback Method
dvisc	0.0000654	Pa×s	973.84	Joback Method
dvisc	0.0000745	Pa×s	932.28	Joback Method

dvisc	0.0000858	Pa×s	890.72	Joback Method
dvisc	0.0001002	Pa×s	849.15	Joback Method
dvisc	0.0001190	Pa×s	807.59	Joback Method
dvisc	0.0001439	Pa×s	766.03	Joback Method
dvisc	0.0001779	Pa×s	724.47	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