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

Inchi: InChI=1S/C12H2Cl8O/c13-3-1-4(14)9(18)12(8(3)17)21-6-2-5(15)7(16)11(20)10(6)19/h1-2
InchiKey: MRHQOXCYYPFGEE-UHFFFAOYSA-N
Formula: C12H2Cl8O
SMILES: Clc1cc(Oc2c(Cl)c(Cl)cc(Cl)c2Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 445.77

Physical Properties

Property code	Value	Unit	Source
gf	-2.50	kJ/mol	Joback Method
hf	-167.85	kJ/mol	Joback Method
hfus	46.57	kJ/mol	Joback Method
hvap	89.64	kJ/mol	Joback Method
log10ws	-10.10		Aqueous Solubility Prediction Method
logp	8.706		Crippen Method
mcvol	236.210	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
tb	889.02	K	Joback Method
tc	1158.50	K	Joback Method
tf	639.59	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.36	J/mol×K	889.02	Joback Method
cpg	469.11	J/mol×K	1113.59	Joback Method
cpg	466.81	J/mol×K	1068.67	Joback Method
cpg	463.70	J/mol×K	1023.76	Joback Method
cpg	459.75	J/mol×K	978.85	Joback Method
cpg	454.97	J/mol×K	933.93	Joback Method
cpg	470.57	J/mol×K	1158.50	Joback Method
dvisc	0.0000851	Pa×s	889.02	Joback Method
dvisc	0.0000982	Pa×s	847.45	Joback Method

dvisc	0.0001150	Pa×s	805.88	Joback Method
dvisc	0.0001370	Pa×s	764.31	Joback Method
dvisc	0.0001664	Pa×s	722.73	Joback Method
dvisc	0.0002071	Pa×s	681.16	Joback Method
dvisc	0.0002652	Pa×s	639.59	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