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

Inchi: InChI=1S/C12HCl9O/c13-2-1-3(5(15)6(16)4(2)14)22-12-10(20)8(18)7(17)9(19)11(12)21/h
InchiKey: FPEYJPVHPGDXDD-UHFFFAOYSA-N
Formula: C12HCl9O
SMILES: Clc1cc(Oc2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 480.22

Physical Properties

Property code	Value	Unit	Source
gf	-24.06	kJ/mol	Joback Method
hf	-195.06	kJ/mol	Joback Method
hfus	50.38	kJ/mol	Joback Method
hvap	94.69	kJ/mol	Joback Method
log10ws	-10.55		Aqueous Solubility Prediction Method
logp	9.360		Crippen Method
mcvol	248.450	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
tb	931.43	K	Joback Method
tc	1202.63	K	Joback Method
tf	682.03	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.40	J/mol×K	931.43	Joback Method
cpg	464.93	J/mol×K	976.63	Joback Method
cpg	468.62	J/mol×K	1021.83	Joback Method
cpg	471.46	J/mol×K	1067.03	Joback Method
cpg	473.44	J/mol×K	1112.23	Joback Method
cpg	474.56	J/mol×K	1157.43	Joback Method
cpg	474.81	J/mol×K	1202.63	Joback Method
dvisc	0.0002168	Pa×s	682.03	Joback Method
dvisc	0.0001726	Pa×s	723.60	Joback Method

dvisc	0.0001408	Pa×s	765.16	Joback Method
dvisc	0.0001173	Pa×s	806.73	Joback Method
dvisc	0.0000995	Pa×s	848.30	Joback Method
dvisc	0.0000857	Pa×s	889.86	Joback Method
dvisc	0.0000748	Pa×s	931.43	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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

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

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