2-Chlorodiphenyl ether

Inchi: InChI=1S/C12H9ClO/c13-11-8-4-5-9-12(11)14-10-6-2-1-3-7-10/h1-9H
InchiKey: IPBRZLMGGXHHMS-UHFFFAOYSA-N
Formula: C12H9ClO
SMILES: Clc1ccccc1Oc1ccccc1
Mol. weight [g/mol]: 204.66

Physical Properties

Property code	Value	Unit	Source
gf	148.42	kJ/mol	Joback Method
hf	22.62	kJ/mol	Joback Method
hfus	19.91	kJ/mol	Joback Method
hvap	54.31	kJ/mol	Joback Method
log10ws	-4.78		Aqueous Solubility Prediction Method
logp	4.132		Crippen Method
mcvol	150.530	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
tb	592.15	K	Joback Method
tc	843.25	K	Joback Method
tf	342.51	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.17	J/mol×K	592.15	Joback Method
cpg	388.95	J/mol×K	801.40	Joback Method
cpg	378.84	J/mol×K	759.55	Joback Method
cpg	367.76	J/mol×K	717.70	Joback Method
cpg	355.65	J/mol×K	675.85	Joback Method
cpg	342.47	J/mol×K	634.00	Joback Method
cpg	398.13	J/mol×K	843.25	Joback Method
dvisc	0.0001652	Pa×s	592.15	Joback Method
dvisc	0.0002065	Pa×s	550.54	Joback Method

dvisc	0.0002678	Pa×s	508.94	Joback Method
dvisc	0.0003636	Pa×s	467.33	Joback Method
dvisc	0.0005242	Pa×s	425.72	Joback Method
dvisc	0.0008182	Pa×s	384.12	Joback Method
dvisc	0.0014227	Pa×s	342.51	Joback Method

Sources

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

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

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