

2,6-Dichlorodiphenyl ether

Inchi:	InChI=1S/C12H8Cl2O/c13-10-7-4-8-11(14)12(10)15-9-5-2-1-3-6-9/h1-8H
InchiKey:	IRLZOQDGEAEIPX-UHFFFAOYSA-N
Formula:	C12H8Cl2O
SMILES:	Clc1cccc(Cl)c1Oc1ccccc1
Mol. weight [g/mol]:	239.10

Physical Properties

Property code	Value	Unit	Source
gf	126.86	kJ/mol	Joback Method
hf	-4.59	kJ/mol	Joback Method
hfus	23.72	kJ/mol	Joback Method
hvap	59.36	kJ/mol	Joback Method
log10ws	-5.06		Aqueous Solubility Prediction Method
logp	4.786		Crippen Method
mcvol	162.770	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
tb	634.56	K	Joback Method
tc	889.75	K	Joback Method
tf	384.95	K	Joback Method
vc	0.608	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.12	J/molxK	634.56	Joback Method
cpg	405.30	J/molxK	847.22	Joback Method
cpg	396.40	J/molxK	804.69	Joback Method
cpg	386.58	J/molxK	762.16	Joback Method
cpg	375.79	J/molxK	719.62	Joback Method
cpg	363.98	J/molxK	677.09	Joback Method
cpg	413.32	J/molxK	889.75	Joback Method
dvisc	0.0001567	Paxs	634.56	Joback Method
dvisc	0.0001927	Paxs	592.96	Joback Method

dvisc	0.0002444	Paxs	551.36	Joback Method
dvisc	0.0003224	Paxs	509.75	Joback Method
dvisc	0.0004466	Paxs	468.15	Joback Method
dvisc	0.0006592	Paxs	426.55	Joback Method
dvisc	0.0010585	Paxs	384.95	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

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