2,4-Dichloro-1-methoxynaphthalene

Inchi: InChI=1S/C11H8Cl2O/c1-14-11-8-5-3-2-4-7(8)9(12)6-10(11)13/h2-6H,1H3
InchiKey: SMNLNHLWUBUPAT-UHFFFAOYSA-N
Formula: C11H8Cl2O
SMILES: COc1c(Cl)cc(Cl)c2ccccc12
Mol. weight [g/mol]: 227.09

Physical Properties

Property code	Value	Unit	Source
gf	103.05	kJ/mol	Joback Method
hf	-40.88	kJ/mol	Joback Method
hfus	23.72	kJ/mol	Joback Method
hvap	57.16	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.155		Crippen Method
mcvol	152.980	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
rinpol	1670.00		NIST Webbook
tb	608.96	K	Joback Method
tc	850.96	K	Joback Method
tf	392.48	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.39	J/mol×K	608.96	Joback Method
cpg	333.75	J/mol×K	649.29	Joback Method
cpg	344.30	J/mol×K	689.63	Joback Method
cpg	354.09	J/mol×K	729.96	Joback Method
cpg	363.17	J/mol×K	770.29	Joback Method
cpg	371.58	J/mol×K	810.62	Joback Method
cpg	379.36	J/mol×K	850.96	Joback Method
dvisc	0.0009974	Pa×s	392.48	Joback Method
dvisc	0.0007397	Pa×s	428.56	Joback Method

dvisc	0.0005747	Pa×s	464.64	Joback Method
dvisc	0.0004631	Pa×s	500.72	Joback Method
dvisc	0.0003841	Pa×s	536.80	Joback Method
dvisc	0.0003262	Pa×s	572.88	Joback Method
dvisc	0.0002824	Pa×s	608.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540282&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume