

3,5-Dichlorophenol, isoBOC

Inchi:	InChI=1S/C11H12Cl2O3/c1-7(2)6-15-11(14)16-10-4-8(12)3-9(13)5-10/h3-5,7H,6H2,1-2H
InchiKey:	FFHCQBFVWVPFTE-UHFFFAOYSA-N
Formula:	C11H12Cl2O3
SMILES:	CC(C)COC(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	263.12

Physical Properties

Property code	Value	Unit	Source
gf	-230.33	kJ/mol	Joback Method
hf	-470.56	kJ/mol	Joback Method
hfus	26.36	kJ/mol	Joback Method
hvap	63.63	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.165		Crippen Method
mcvol	179.880	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
rinpol	1674.00		NIST Webbook
rinpol	1674.00		NIST Webbook
tb	660.85	K	Joback Method
tc	881.40	K	Joback Method
tf	404.42	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.47	J/molxK	660.85	Joback Method
cpg	475.17	J/molxK	844.64	Joback Method
cpg	465.99	J/molxK	807.88	Joback Method
cpg	456.03	J/molxK	771.12	Joback Method
cpg	445.29	J/molxK	734.37	Joback Method
cpg	433.77	J/molxK	697.61	Joback Method
cpg	483.57	J/molxK	881.40	Joback Method
dvisc	0.0001298	Paxs	660.85	Joback Method

dvisc	0.0001626	Paxs	618.11	Joback Method
dvisc	0.0002104	Paxs	575.37	Joback Method
dvisc	0.0002839	Paxs	532.63	Joback Method
dvisc	0.0004037	Paxs	489.90	Joback Method
dvisc	0.0006138	Paxs	447.16	Joback Method
dvisc	0.0010197	Paxs	404.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R235108&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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

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