2,3,4-Trichlorophenol, isoBOC

Inchi: InChI=1S/C11H11Cl3O3/c1-6(2)5-16-11(15)17-8-4-3-7(12)9(13)10(8)14/h3-4,6H,5H2,1-2
InchiKey: UFAMQNYUAIFDGK-UHFFFAOYSA-N
Formula: C11H11Cl3O3
SMILES: CC(C)COC(=O)Oc1ccc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 297.56

Physical Properties

Property code	Value	Unit	Source
gf	-251.89	kJ/mol	Joback Method
hf	-497.77	kJ/mol	Joback Method
hfus	30.16	kJ/mol	Joback Method
hvap	68.67	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.818		Crippen Method
mcvol	192.120	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	1878.00		NIST Webbook
rinpol	1878.00		NIST Webbook
tb	703.26	K	Joback Method
tc	927.66	K	Joback Method
tf	446.86	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.25	J/mol×K	703.26	Joback Method
cpg	491.50	J/mol×K	890.26	Joback Method
cpg	483.43	J/mol×K	852.86	Joback Method
cpg	474.56	J/mol×K	815.46	Joback Method
cpg	464.90	J/mol×K	778.06	Joback Method
cpg	454.46	J/mol×K	740.66	Joback Method
cpg	498.78	J/mol×K	927.66	Joback Method
dvisc	0.0001172	Pa×s	703.26	Joback Method

dvisc	0.0001444	Pa×s	660.53	Joback Method
dvisc	0.0001831	Pa×s	617.79	Joback Method
dvisc	0.0002406	Pa×s	575.06	Joback Method
dvisc	0.0003302	Pa×s	532.33	Joback Method
dvisc	0.0004789	Pa×s	489.59	Joback Method
dvisc	0.0007459	Pa×s	446.86	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R234883&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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