Carbonic acid, isobutyl 3,4-dichlorophenyl ester

Other names: 3,4-Dichlorophenol, isoBOC
Inchi: InChI=1S/C11H12Cl2O3/c1-7(2)6-15-11(14)16-8-3-4-9(12)10(13)5-8/h3-5,7H,6H2,1-2H3
InchiKey: MZLYKZNYZWBUCP-UHFFFAOYSA-N
Formula: C11H12Cl2O3
SMILES: CC(C)COC(=O)Oc1ccc(Cl)c(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	1746.00		NIST Webbook
rinpol	1722.00		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/mol×K	660.85	Joback Method
cpg	475.17	J/mol×K	844.64	Joback Method
cpg	465.99	J/mol×K	807.88	Joback Method
cpg	456.03	J/mol×K	771.12	Joback Method
cpg	445.29	J/mol×K	734.37	Joback Method
cpg	433.77	J/mol×K	697.61	Joback Method
cpg	483.57	J/mol×K	881.40	Joback Method

dvisc	0.0001298	Pa×s	660.85	Joback Method
dvisc	0.0001626	Pa×s	618.11	Joback Method
dvisc	0.0002104	Pa×s	575.37	Joback Method
dvisc	0.0002839	Pa×s	532.63	Joback Method
dvisc	0.0004037	Pa×s	489.90	Joback Method
dvisc	0.0006138	Pa×s	447.16	Joback Method
dvisc	0.0010197	Pa×s	404.42	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=U357837&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