1,3-Dichloroisopropyl isobutyrate

Inchi: InChI=1S/C7H12Cl2O2/c1-5(2)6(10)11-7(3,9)4-8/h5H,4H2,1-3H3
InchiKey: KYRAJGTUGZGYCT-UHFFFAOYSA-N
Formula: C7H12Cl2O2
SMILES: CC(C)C(=O)OC(C)(Cl)CCl
Mol. weight [g/mol]: 199.07

Physical Properties

Property code	Value	Unit	Source
gf	-249.32	kJ/mol	Joback Method
hf	-478.12	kJ/mol	Joback Method
hfus	14.13	kJ/mol	Joback Method
hvap	47.42	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.379		Crippen Method
mcvol	141.410	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	1158.00		NIST Webbook
rinpol	1158.00		NIST Webbook
tb	507.04	K	Joback Method
tc	711.27	K	Joback Method
tf	288.07	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.39	J/mol×K	507.04	Joback Method
cpg	305.93	J/mol×K	541.08	Joback Method
cpg	316.82	J/mol×K	575.12	Joback Method
cpg	327.06	J/mol×K	609.16	Joback Method
cpg	336.69	J/mol×K	643.19	Joback Method
cpg	345.73	J/mol×K	677.23	Joback Method
cpg	354.21	J/mol×K	711.27	Joback Method
dvisc	0.0048226	Pa×s	288.07	Joback Method

dvisc	0.0022450	Pa×s	324.56	Joback Method
dvisc	0.0012198	Pa×s	361.06	Joback Method
dvisc	0.0007413	Pa×s	397.55	Joback Method
dvisc	0.0004899	Pa×s	434.05	Joback Method
dvisc	0.0003452	Pa×s	470.54	Joback Method
dvisc	0.0002558	Pa×s	507.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R150240&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

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