2,3-Dichloropropyl isopentanoate

Other names: 1-Propanol, 2,3-dichloro, 3-methylbutanoate
Inchi: InChI=1S/C8H14Cl2O2/c1-6(2)3-8(11)12-5-7(10)4-9/h6-7H,3-5H2,1-2H3
InchiKey: PFULRUXYGVMVTG-UHFFFAOYSA-N
Formula: C8H14Cl2O2
SMILES: CC(C)CC(=O)OCC(Cl)CCl
Mol. weight [g/mol]: 213.10

Physical Properties

Property code	Value	Unit	Source
gf	-246.18	kJ/mol	Joback Method
hf	-495.29	kJ/mol	Joback Method
hfus	20.61	kJ/mol	Joback Method
hvap	50.55	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.422		Crippen Method
mcvol	155.500	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1271.00		NIST Webbook
rinpol	1271.00		NIST Webbook
tb	532.71	K	Joback Method
tc	726.47	K	Joback Method
tf	281.92	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.03	J/mol×K	532.71	Joback Method
cpg	347.00	J/mol×K	565.00	Joback Method
cpg	358.41	J/mol×K	597.30	Joback Method
cpg	369.28	J/mol×K	629.59	Joback Method
cpg	379.60	J/mol×K	661.88	Joback Method
cpg	389.40	J/mol×K	694.18	Joback Method
cpg	398.67	J/mol×K	726.47	Joback Method

dvisc	0.0049812	Pa×s	281.92	Joback Method
dvisc	0.0021345	Pa×s	323.72	Joback Method
dvisc	0.0011103	Pa×s	365.52	Joback Method
dvisc	0.0006604	Pa×s	407.32	Joback Method
dvisc	0.0004327	Pa×s	449.11	Joback Method
dvisc	0.0003047	Pa×s	490.91	Joback Method
dvisc	0.0002267	Pa×s	532.71	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R34141&Units=SI

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