1-Propanol, 2,3-dichloro, butanoate

Other names: 2,3-Dichloropropyl butyrate
Inchi: InChI=1S/C7H12Cl2O2/c1-2-3-7(10)11-5-6(9)4-8/h6H,2-5H2,1H3
InchiKey: KKIRBVXTFOTIRJ-UHFFFAOYSA-N
Formula: C7H12Cl2O2
SMILES: CCCC(=O)OCC(Cl)CCl
Mol. weight [g/mol]: 199.07

Physical Properties

Property code	Value	Unit	Source
gf	-252.16	kJ/mol	Joback Method
hf	-469.37	kJ/mol	Joback Method
hfus	21.54	kJ/mol	Joback Method
hvap	48.71	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	2.176		Crippen Method
mcvol	141.410	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	1220.00		NIST Webbook
tb	510.27	K	Joback Method
tc	702.42	K	Joback Method
tf	285.65	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.96	J/mol×K	510.27	Joback Method
cpg	339.62	J/mol×K	670.39	Joback Method
cpg	330.81	J/mol×K	638.37	Joback Method
cpg	321.54	J/mol×K	606.34	Joback Method
cpg	311.82	J/mol×K	574.32	Joback Method
cpg	301.62	J/mol×K	542.29	Joback Method
cpg	347.98	J/mol×K	702.42	Joback Method
dvisc	0.0002658	Pa×s	510.27	Joback Method

dvisc	0.0003470	Pa×s	472.83	Joback Method
dvisc	0.0004742	Pa×s	435.40	Joback Method
dvisc	0.0006874	Pa×s	397.96	Joback Method
dvisc	0.0010763	Pa×s	360.52	Joback Method
dvisc	0.0018698	Pa×s	323.09	Joback Method
dvisc	0.0037541	Pa×s	285.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R34169&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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