2,2-Dimethylpropanoic acid, 3-chloroprop-2-enyl ester

Inchi: InChI=1S/C8H13ClO2/c1-8(2,3)7(10)11-6-4-5-9/h4-5H,6H2,1-3H3/b5-4+

InchiKey: HEINMRDBMAQWSG-SNAWJCMRSA-N

Formula: C8H13ClO2

SMILES: CC(C)(C)C(=O)OCC=CCl

Mol. weight [g/mol]: 176.64

Physical Properties

Property code	Value	Unit	Source
gf	-146.31	kJ/mol	Joback Method
hf	-360.52	kJ/mol	Joback Method
hfus	16.25	kJ/mol	Joback Method
hvap	45.61	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.328		Crippen Method
mcvol	138.960	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
tb	497.09	K	Joback Method
tc	698.01	K	Joback Method
tf	279.34	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.37	J/mol×K	497.09	Joback Method
cpg	305.75	J/mol×K	530.58	Joback Method
cpg	317.41	J/mol×K	564.06	Joback Method
cpg	328.39	J/mol×K	597.55	Joback Method
cpg	338.71	J/mol×K	631.04	Joback Method
cpg	348.41	J/mol×K	664.52	Joback Method
cpg	357.52	J/mol×K	698.01	Joback Method
dvisc	0.0037158	Pa×s	279.34	Joback Method
dvisc	0.0017567	Pa×s	315.63	Joback Method
dvisc	0.0009692	Pa×s	351.92	Joback Method

dvisc	0.0005977	Pa×s	388.22	Joback Method
dvisc	0.0004003	Pa×s	424.51	Joback Method
dvisc	0.0002856	Pa×s	460.80	Joback Method
dvisc	0.0002140	Pa×s	497.09	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=U299339&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume