3-Methyl-2-butenoic acid, 3-chloroprop-2-enyl ester

Inchi: InChI=1S/C8H11ClO2/c1-7(2)6-8(10)11-5-3-4-9/h3-4,6H,5H2,1-2H3/b4-3+
InchiKey: UHEWJISEFLFVKJ-ONEGZZNKSA-N
Formula: C8H11ClO2
SMILES: CC(C)=CC(=O)OCC=CCl
Mol. weight [g/mol]: 174.62

Physical Properties

Property code	Value	Unit	Source
gf	-77.48	kJ/mol	Joback Method
hf	-244.34	kJ/mol	Joback Method
hfus	22.55	kJ/mol	Joback Method
hvap	46.94	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.248		Crippen Method
mcvol	134.660	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
rinpol	1180.00		NIST Webbook
rinpol	1180.00		NIST Webbook
tb	504.36	K	Joback Method
tc	705.80	K	Joback Method
tf	257.88	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.19	J/mol×K	504.36	Joback Method
cpg	283.26	J/mol×K	537.93	Joback Method
cpg	293.73	J/mol×K	571.51	Joback Method
cpg	303.62	J/mol×K	605.08	Joback Method
cpg	312.96	J/mol×K	638.65	Joback Method
cpg	321.78	J/mol×K	672.22	Joback Method
cpg	330.11	J/mol×K	705.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299318&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
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