3-Chloropropionic acid, 3-methylbut-2-enyl ester

Inchi: InChI=1S/C8H13ClO2/c1-7(2)4-6-11-8(10)3-5-9/h4H,3,5-6H2,1-2H3
InchiKey: JQSINDIMIDHUQE-UHFFFAOYSA-N
Formula: C8H13ClO2
SMILES: CC(C)=CCOC(=O)CCCl
Mol. weight [g/mol]: 176.64

Physical Properties

Property code	Value	Unit	Source
gf	-157.70	kJ/mol	Joback Method
hf	-361.56	kJ/mol	Joback Method
hfus	22.35	kJ/mol	Joback Method
hvap	46.98	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	2.125		Crippen Method
mcvol	138.960	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	1168.00		NIST Webbook
tb	500.20	K	Joback Method
tc	692.68	K	Joback Method
tf	262.96	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.98	J/mol×K	500.20	Joback Method
cpg	301.57	J/mol×K	532.28	Joback Method
cpg	312.61	J/mol×K	564.36	Joback Method
cpg	323.13	J/mol×K	596.44	Joback Method
cpg	333.14	J/mol×K	628.52	Joback Method
cpg	342.66	J/mol×K	660.60	Joback Method
cpg	351.69	J/mol×K	692.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299213&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
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