Z-Acetic acid 3-chloro-2-methyl-allyl ester

Inchi: InChI=1S/C6H9ClO2/c1-5(3-7)4-9-6(2)8/h3H,4H2,1-2H3/b5-3-
InchiKey: XNYISLNQOFYBEH-HYXAFXHYSA-N
Formula: C6H9ClO2
SMILES: CC(=O)OCC(C)=CCl
Mol. weight [g/mol]: 148.59

Physical Properties

Property code	Value	Unit	Source
gf	-174.54	kJ/mol	Joback Method
hf	-320.28	kJ/mol	Joback Method
hfus	17.17	kJ/mol	Joback Method
hvap	42.53	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.692		Crippen Method
mcvol	110.780	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
rinpol	917.70		NIST Webbook
ripol	1382.40		NIST Webbook
tb	454.44	K	Joback Method
tc	651.59	K	Joback Method
tf	240.42	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.20	J/mol×K	454.44	Joback Method
cpg	217.48	J/mol×K	487.30	Joback Method
cpg	226.33	J/mol×K	520.16	Joback Method
cpg	234.76	J/mol×K	553.01	Joback Method
cpg	242.79	J/mol×K	585.87	Joback Method
cpg	250.42	J/mol×K	618.73	Joback Method
cpg	257.66	J/mol×K	651.59	Joback Method

Sources

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=R154237&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume