Z-Thioacetic acid S-(3-chloro-2-methyl-allyl) ester

Inchi: InChI=1S/C6H9ClOS/c1-5(3-7)4-9-6(2)8/h3H,4H2,1-2H3/b5-3-
InchiKey: BMVLILHIBODFDS-HYXAFXHYSA-N
Formula: C6H9ClOS
SMILES: CC(=O)SCC(C)=CCl
Mol. weight [g/mol]: 164.65

Physical Properties

Property code	Value	Unit	Source
gf	-36.42	kJ/mol	Joback Method
hf	-146.19	kJ/mol	Joback Method
hfus	20.11	kJ/mol	Joback Method
hvap	46.94	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.409		Crippen Method
mcvol	121.260	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
rinpol	1130.80		NIST Webbook
ripol	1567.40		NIST Webbook
tb	500.80	K	Joback Method
tc	721.59	K	Joback Method
tf	252.59	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.77	J/mol×K	500.80	Joback Method
cpg	239.68	J/mol×K	537.60	Joback Method
cpg	249.01	J/mol×K	574.40	Joback Method
cpg	257.76	J/mol×K	611.19	Joback Method
cpg	265.98	J/mol×K	647.99	Joback Method
cpg	273.67	J/mol×K	684.79	Joback Method
cpg	280.87	J/mol×K	721.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R154242&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume