

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

Inchi:	InChI=1S/C6H9CIOS/c1-5(3-7)4-9-6(2)8/h3H,4H2,1-2H3/b5-3+
InchiKey:	BMVLILHIBODFDS-HWKANZROSA-N
Formula:	C6H9CIOS
SMILES:	CC(=O)SCC(C)=CCI
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
mvol	121.260	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
rinpol	1146.10		NIST Webbook
ripol	1623.60		NIST Webbook
tb	500.80	K	Joback Method
tc	721.59	K	Joback Method
tf	252.59	K	Joback Method
vc	0.462	m <sup>3</sup> /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

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R154024&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R154024&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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