

# Ethanethioic acid, chloro-, S-(1-hydroxy-1-methylethyl) ester

Inchi:	InChI=1S/C5H9ClO2S/c1-5(2,8)9-4(7)3-6/h8H,3H2,1-2H3
InchiKey:	GDDZVLZUEQMTLZ-UHFFFAOYSA-N
Formula:	C5H9ClO2S
SMILES:	CC(C)(O)SC(=O)CCl
Mol. weight [g/mol]:	168.64
CAS:	37960-78-4

## Physical Properties

Property code	Value	Unit	Source
gf	-250.49	kJ/mol	Joback Method
hf	-393.96	kJ/mol	Joback Method
hfus	15.31	kJ/mol	Joback Method
hvap	60.06	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.213		Crippen Method
mcvol	117.340	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
tb	562.83	K	Joback Method
tc	770.73	K	Joback Method
tf	323.60	K	Joback Method
vc	0.432	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.14	J/molxK	562.83	Joback Method
cpg	259.36	J/molxK	597.48	Joback Method
cpg	267.03	J/molxK	632.13	Joback Method
cpg	274.18	J/molxK	666.78	Joback Method
cpg	280.84	J/molxK	701.43	Joback Method
cpg	287.02	J/molxK	736.08	Joback Method
cpg	292.75	J/molxK	770.73	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<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=C37960784&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C37960784&amp;Units=SI</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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