

# Ethanedithioic acid, S-(1-hydroxy-1-methylethyl) ester

Inchi:	InChI=1S/C5H10O2S/c1-4(6)8-5(2,3)7/h7H,1-3H3
InchiKey:	NMSBMSLXIQNADU-UHFFFAOYSA-N
Formula:	C5H10O2S
SMILES:	CC(=O)SC(C)(C)O
Mol. weight [g/mol]:	134.20
CAS:	37960-77-3

## Physical Properties

Property code	Value	Unit	Source
gf	-238.56	kJ/mol	Joback Method
hf	-378.22	kJ/mol	Joback Method
hfus	11.11	kJ/mol	Joback Method
hvap	55.67	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	0.994		Crippen Method
mcvol	105.100	ml/mol	McGowan Method
pc	4403.25	kPa	Joback Method
tb	525.40	K	Joback Method
tc	728.69	K	Joback Method
tf	293.68	K	Joback Method
vc	0.384	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.48	J/mol×K	525.40	Joback Method
cpg	238.39	J/mol×K	559.28	Joback Method
cpg	246.75	J/mol×K	593.16	Joback Method
cpg	254.60	J/mol×K	627.05	Joback Method
cpg	261.95	J/mol×K	660.93	Joback Method
cpg	268.83	J/mol×K	694.81	Joback Method
cpg	275.26	J/mol×K	728.69	Joback Method

# Sources

<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=C37960773&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C37960773&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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