

# Propanoic acid, 3-mercapto-, ethyl ester

<b>Other names:</b>	Propionic acid, 3-mercapto-, ethyl ester Ethyl «beta»-mercaptopropionate Ethyl 3-mercaptopropionate 3-Mercaptopropanoic acid ethyl ester
<b>Inchi:</b>	InChI=1S/C5H10O2S/c1-2-7-5(6)3-4-8/h8H,2-4H2,1H3
<b>InchiKey:</b>	CJQWLNNCQIHKHP-UHFFFAOYSA-N
<b>Formula:</b>	C5H10O2S
<b>SMILES:</b>	CCOC(=O)CCS
<b>Mol. weight [g/mol]:</b>	134.20
<b>CAS:</b>	5466-06-8

## Physical Properties

Property code	Value	Unit	Source
gf	-213.31	kJ/mol	Joback Method
hf	-352.85	kJ/mol	Joback Method
hfus	15.53	kJ/mol	Joback Method
hvap	42.62	kJ/mol	Joback Method
log10ws	-0.85		Crippen Method
logp	0.869		Crippen Method
mcvol	105.100	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
tb	452.95	K	Joback Method
tc	654.90	K	Joback Method
tf	254.73	K	Joback Method
vc	0.394	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.20	J/molxK	452.95	Joback Method
cpg	213.49	J/molxK	486.61	Joback Method
cpg	222.42	J/molxK	520.27	Joback Method
cpg	231.01	J/molxK	553.93	Joback Method
cpg	239.23	J/molxK	587.58	Joback Method

cpg	247.10	J/mol×K	621.24	Joback Method
cpg	254.60	J/mol×K	654.90	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	348.70	K	1.30	NIST Webbook

## Sources

<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=C5466068&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5466068&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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