

# 2-Propenoic acid, 3-(methylthio)-, methyl ester

<b>Other names:</b>	Methyl 3-(methylthio)-2-propenoate Methyl 3-(methylsulfanyl)-2-propenoate
<b>Inchi:</b>	InChI=1S/C5H8O2S/c1-7-5(6)3-4-8-2/h3-4H,1-2H3/b4-3-
<b>InchiKey:</b>	KAFIOMPFBSDFP-ARJAWSKDSA-N
<b>Formula:</b>	C5H8O2S
<b>SMILES:</b>	COC(=O)C=CSC
<b>Mol. weight [g/mol]:</b>	132.18
<b>CAS:</b>	13733-57-8

## Physical Properties

Property code	Value	Unit	Source
gf	-129.36	kJ/mol	Joback Method
hf	-232.24	kJ/mol	Joback Method
hfus	15.82	kJ/mol	Joback Method
hvap	42.66	kJ/mol	Joback Method
log10ws	-1.01		Crippen Method
logp	1.036		Crippen Method
mcvol	100.800	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
rinpol	1063.00		NIST Webbook
rinpol	1063.00		NIST Webbook
ripol	1647.00		NIST Webbook
tb	463.03	K	Joback Method
tc	675.06	K	Joback Method
tf	247.59	K	Joback Method
vc	0.373	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.44	J/mol×K	463.03	Joback Method
cpg	197.25	J/mol×K	498.37	Joback Method
cpg	205.66	J/mol×K	533.71	Joback Method
cpg	213.69	J/mol×K	569.05	Joback Method

cpg	221.33	J/mol×K	604.38	Joback Method
cpg	228.58	J/mol×K	639.72	Joback Method
cpg	235.46	J/mol×K	675.06	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=C13733578&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13733578&amp;Units=SI</a>
<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>

## 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>rinpol:</b>	Non-polar retention indices
<b>ripol:</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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