

# 3-(methylthio)propyl acetate

<b>Other names:</b>	Methionol, acetate 1-Propanol, 3-(methylthio)-, acetate
<b>Inchi:</b>	InChI=1S/C6H12O2S/c1-6(7)8-4-3-5-9-2/h3-5H2,1-2H3
<b>InchiKey:</b>	LPZQTNIAYMRVMF-UHFFFAOYSA-N
<b>Formula:</b>	C6H12O2S
<b>SMILES:</b>	CSCCCOC(C)=O
<b>Mol. weight [g/mol]:</b>	148.22
<b>CAS:</b>	16630-55-0

## Physical Properties

Property code	Value	Unit	Source
gf	-201.16	kJ/mol	Joback Method
hf	-370.10	kJ/mol	Joback Method
hfus	18.21	kJ/mol	Joback Method
hvap	44.92	kJ/mol	Joback Method
log10ws	-1.08		Crippen Method
logp	1.303		Crippen Method
mcvol	119.190	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
rinpol	1123.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1133.00		NIST Webbook
ripol	1613.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1633.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1627.00		NIST Webbook
tb	481.75	K	Joback Method
tc	681.10	K	Joback Method
tf	263.94	K	Joback Method
vc	0.450	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.41	J/mol×K	481.75	Joback Method
cpg	256.09	J/mol×K	514.98	Joback Method
cpg	266.37	J/mol×K	548.20	Joback Method
cpg	276.25	J/mol×K	581.43	Joback Method
cpg	285.71	J/mol×K	614.65	Joback Method
cpg	294.75	J/mol×K	647.88	Joback Method
cpg	303.37	J/mol×K	681.10	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=C16630550&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16630550&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>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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