

# 5-Methyl-4-mercaptohexyl-2-acetate, # 2

<b>Inchi:</b>	InChI=1S/C9H18O2S/c1-6(2)9(12)5-7(3)11-8(4)10/h6-7,9,12H,5H2,1-4H3
<b>InchiKey:</b>	XCOUODRDDWCWCD-UHFFFAOYSA-N
<b>Formula:</b>	C9H18O2S
<b>SMILES:</b>	CC(=O)OC(C)CC(S)C(C)C
<b>Mol. weight [g/mol]:</b>	190.30

## Physical Properties

Property code	Value	Unit	Source
gf	-186.95	kJ/mol	Joback Method
hf	-451.25	kJ/mol	Joback Method
hfus	15.33	kJ/mol	Joback Method
hvap	50.36	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.283		Crippen Method
mcvol	161.460	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
rinsol	1238.00		NIST Webbook
tb	543.15	K	Joback Method
tc	747.37	K	Joback Method
tf	254.81	K	Joback Method
vc	0.600	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.02	J/molxK	543.15	Joback Method
cpg	390.80	J/molxK	577.19	Joback Method
cpg	404.88	J/molxK	611.22	Joback Method
cpg	418.25	J/molxK	645.26	Joback Method
cpg	430.94	J/molxK	679.30	Joback Method
cpg	442.94	J/molxK	713.34	Joback Method
cpg	454.27	J/molxK	747.37	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=R603244&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R603244&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>rinpola:</b>	Non-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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