

# 4-Mercaptononyl-2-acetate, # 2

<b>Inchi:</b>	InChI=1S/C11H22O2S/c1-4-5-6-7-11(14)8-9(2)13-10(3)12/h9,11,14H,4-8H2,1-3H3
<b>InchiKey:</b>	ATUWCVJQUQRXHL-UHFFFAOYSA-N
<b>Formula:</b>	C11H22O2S
<b>SMILES:</b>	CCCCC(S)CC(C)OC(C)=O
<b>Mol. weight [g/mol]:</b>	218.36

## Physical Properties

Property code	Value	Unit	Source
gf	-167.67	kJ/mol	Joback Method
hf	-487.25	kJ/mol	Joback Method
hfus	24.03	kJ/mol	Joback Method
hvap	55.20	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.207		Crippen Method
mvol	189.640	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rmpol	1438.00		NIST Webbook
tb	589.35	K	Joback Method
tc	783.94	K	Joback Method
tf	292.35	K	Joback Method
vc	0.718	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.56	J/molxK	589.35	Joback Method
cpg	488.44	J/molxK	621.78	Joback Method
cpg	503.56	J/molxK	654.21	Joback Method
cpg	517.93	J/molxK	686.64	Joback Method
cpg	531.56	J/molxK	719.08	Joback Method
cpg	544.48	J/molxK	751.51	Joback Method
cpg	556.68	J/molxK	783.94	Joback Method

# 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=R603120&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R603120&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>
<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>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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