

# 2-Mercaptohexyl-4-acetate, # 2

<b>Inchi:</b>	InChI=1S/C8H16O2S/c1-4-8(5-6(2)11)10-7(3)9/h6,8,11H,4-5H2,1-3H3
<b>InchiKey:</b>	JVSSZFATQMMTDW-UHFFFAOYSA-N
<b>Formula:</b>	C8H16O2S
<b>SMILES:</b>	CCC(CC(C)S)OC(C)=O
<b>Mol. weight [g/mol]:</b>	176.28

## Physical Properties

Property code	Value	Unit	Source
gf	-192.93	kJ/mol	Joback Method
hf	-425.33	kJ/mol	Joback Method
hfus	16.26	kJ/mol	Joback Method
hvap	48.52	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.036		Crippen Method
mvol	147.370	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1157.00		NIST Webbook
rinpol	1157.00		NIST Webbook
tb	520.71	K	Joback Method
tc	723.56	K	Joback Method
tf	258.54	K	Joback Method
vc	0.549	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.93	J/mol×K	520.71	Joback Method
cpg	343.43	J/mol×K	554.52	Joback Method
cpg	356.32	J/mol×K	588.33	Joback Method
cpg	368.60	J/mol×K	622.14	Joback Method
cpg	380.27	J/mol×K	655.94	Joback Method
cpg	391.34	J/mol×K	689.75	Joback Method
cpg	401.82	J/mol×K	723.56	Joback Method

# Sources

<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>
<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=R602845&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R602845&amp;Units=SI</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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