

# 2-[Isopropylthio]ethanal

<b>Inchi:</b>	InChI=1S/C5H10OS/c1-5(2)7-4-3-6/h3,5H,4H2,1-2H3
<b>InchiKey:</b>	ATGYXQXFCDNCEM-UHFFFAOYSA-N
<b>Formula:</b>	C5H10OS
<b>SMILES:</b>	CC(C)SCC=O
<b>Mol. weight [g/mol]:</b>	118.20

## Physical Properties

Property code	Value	Unit	Source
gf	-77.62	kJ/mol	Joback Method
hf	-195.52	kJ/mol	Joback Method
hfus	11.60	kJ/mol	Joback Method
hvap	39.87	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.327		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	3911.14	kPa	Joback Method
ripol	1391.00		NIST Webbook
tb	430.80	K	Joback Method
tc	633.07	K	Joback Method
tf	207.51	K	Joback Method
vc	0.381	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.63	J/molxK	430.80	Joback Method
cpg	196.13	J/molxK	464.51	Joback Method
cpg	205.22	J/molxK	498.22	Joback Method
cpg	213.91	J/molxK	531.93	Joback Method
cpg	222.20	J/molxK	565.64	Joback Method
cpg	230.09	J/molxK	599.36	Joback Method
cpg	237.59	J/molxK	633.07	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R402150&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R402150&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>
<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>

# 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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