

# 1-Hexanethiol, 2-ethyl-

<b>Other names:</b>	2-Ethyl-1-hexanethiol 2-ethylhexane-1-thiol
<b>Inchi:</b>	InChI=1S/C8H18S/c1-3-5-6-8(4-2)7-9/h8-9H,3-7H2,1-2H3
<b>InchiKey:</b>	UCJMHYXRQZYNNL-UHFFFAOYSA-N
<b>Formula:</b>	C8H18S
<b>SMILES:</b>	CCCCCC(CC)CS
<b>Mol. weight [g/mol]:</b>	146.29
<b>CAS:</b>	7341-17-5

## Physical Properties

Property code	Value	Unit	Source
gf	43.43	kJ/mol	Joback Method
hf	-175.25	kJ/mol	Joback Method
hfus	17.00	kJ/mol	Joback Method
hvap	39.75	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	3.133		Crippen Method
mvol	139.930	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
tb	444.86	K	Joback Method
tc	634.61	K	Joback Method
tf	201.38	K	Joback Method
vc	0.531	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.76	J/mol×K	444.86	Joback Method
cpg	299.03	J/mol×K	476.48	Joback Method
cpg	312.67	J/mol×K	508.11	Joback Method
cpg	325.72	J/mol×K	539.73	Joback Method
cpg	338.18	J/mol×K	571.36	Joback Method
cpg	350.07	J/mol×K	602.98	Joback Method
cpg	361.41	J/mol×K	634.61	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C7341175&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7341175&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>hvp:</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>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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