

# 2-Hydroxyethyl propyl sulfide

<b>Other names:</b>	2-Hydroxyethyl n-propyl sulfide «beta»-Hydroxyethyl-n-propyl sulfide Ethanol, 2-(propylthio)- 2-(propylthio)ethanol
<b>Inchi:</b>	InChI=1S/C5H12OS/c1-2-4-7-5-3-6/h6H,2-5H2,1H3
<b>InchiKey:</b>	KCWXXYQPUDKBX-UHFFFAOYSA-N
<b>Formula:</b>	C5H12OS
<b>SMILES:</b>	CCCSCCO
<b>Mol. weight [g/mol]:</b>	120.21
<b>CAS:</b>	22812-90-4

## Physical Properties

Property code	Value	Unit	Source
gf	-112.48	kJ/mol	Joback Method
hf	-256.89	kJ/mol	Joback Method
hfus	16.92	kJ/mol	Joback Method
hvap	50.22	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	1.122		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	474.76	K	Joback Method
tc	656.94	K	Joback Method
tf	241.33	K	Joback Method
vc	0.389	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.57	J/molxK	474.76	Joback Method
cpg	222.54	J/molxK	505.12	Joback Method
cpg	231.16	J/molxK	535.49	Joback Method
cpg	239.43	J/molxK	565.85	Joback Method
cpg	247.36	J/molxK	596.22	Joback Method

cpg	254.95	J/mol×K	626.58	Joback Method
cpg	262.20	J/mol×K	656.94	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C22812904&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22812904&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>mcpv:</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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