

# Propane, 1-(ethynylsulfinyl)-

<b>Other names:</b>	Propyl ethynyl sulfoxide
<b>Inchi:</b>	InChI=1S/C5H8OS/c1-3-5-7(6)4-2/h2H,3,5H2,1H3
<b>InchiKey:</b>	OXLSTZIMSSWILC-UHFFFAOYSA-N
<b>Formula:</b>	C5H8OS
<b>SMILES:</b>	C#CS(=O)CCC
<b>Mol. weight [g/mol]:</b>	116.18
<b>CAS:</b>	121564-27-0

## Physical Properties

Property code	Value	Unit	Source
gf	-3.42	kJ/mol	Joback Method
hf	-60.37	kJ/mol	Joback Method
hfus	19.44	kJ/mol	Joback Method
hvap	39.31	kJ/mol	Joback Method
log10ws	-0.84		Crippen Method
logp	0.736		Crippen Method
mcvol	94.930	ml/mol	McGowan Method
pc	4665.71	kPa	Joback Method
tb	362.20	K	Joback Method
tc	551.26	K	Joback Method
tf	229.56	K	Joback Method
vc	0.367	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.95	J/mol×K	362.20	Joback Method
cpg	167.25	J/mol×K	393.71	Joback Method
cpg	175.23	J/mol×K	425.22	Joback Method
cpg	182.87	J/mol×K	456.73	Joback Method
cpg	190.20	J/mol×K	488.24	Joback Method
cpg	197.20	J/mol×K	519.75	Joback Method
cpg	203.90	J/mol×K	551.26	Joback Method

# Sources

<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=C121564270&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C121564270&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>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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