

# Propyl 1-propenyl disulfide

<b>Other names:</b>	Disulfide, 1-propenyl propyl Propyl 1-propenyl disulfide, (Z)- Propyl propenyl disulphide 1-propenyl propyl disulfide prop-1-enyl propyl disulphide
<b>Inchi:</b>	InChI=1S/C6H12S2/c1-3-5-7-8-6-4-2/h3,5H,4,6H2,1-2H3
<b>InchiKey:</b>	AAPBYIVJOWCMGH-UHFFFAOYSA-N
<b>Formula:</b>	C6H12S2
<b>SMILES:</b>	CC=CSSCCC
<b>Mol. weight [g/mol]:</b>	148.29
<b>CAS:</b>	5905-46-4

## Physical Properties

Property code	Value	Unit	Source
gf	146.10	kJ/mol	Joback Method
hf	33.79	kJ/mol	Joback Method
hfus	19.76	kJ/mol	Joback Method
hvap	42.54	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.311		Crippen Method
mcvol	123.800	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
rinpol	1116.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1102.00		NIST Webbook
ripol	1436.00		NIST Webbook
tb	478.40	K	Joback Method
tc	701.27	K	Joback Method
tf	221.10	K	Joback Method
vc	0.460	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.88	J/mol×K	478.40	Joback Method
cpg	248.67	J/mol×K	515.55	Joback Method
cpg	259.83	J/mol×K	552.69	Joback Method
cpg	270.40	J/mol×K	589.84	Joback Method
cpg	280.37	J/mol×K	626.98	Joback Method
cpg	289.77	J/mol×K	664.13	Joback Method
cpg	298.61	J/mol×K	701.27	Joback Method

## Sources

<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=C5905464&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5905464&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>

## 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>rinpol:</b>	Non-polar retention indices
<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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