

# (Z)-1-(Prop-1-en-1-yl)-3-propyltrisulfane

<b>Inchi:</b>	InChI=1S/C6H12S3/c1-3-5-7-9-8-6-4-2/h3,5H,4,6H2,1-2H3/b5-3-
<b>InchiKey:</b>	CKVNYTRYOFXVGM-HYXAFXHYSA-N
<b>Formula:</b>	C6H12S3
<b>SMILES:</b>	CC=CSSSCCC
<b>Mol. weight [g/mol]:</b>	180.35
<b>CAS:</b>	23838-26-8

## Physical Properties

Property code	Value	Unit	Source
gf	179.22	kJ/mol	Joback Method
hf	75.66	kJ/mol	Joback Method
hfus	23.89	kJ/mol	Joback Method
hvap	49.36	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.960		Crippen Method
mvol	140.150	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
rinpol	1331.30		NIST Webbook
tb	547.18	K	Joback Method
tc	792.12	K	Joback Method
tf	255.50	K	Joback Method
vc	0.513	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.26	J/molxK	547.18	Joback Method
cpg	294.48	J/molxK	588.00	Joback Method
cpg	305.95	J/molxK	628.83	Joback Method
cpg	316.70	J/molxK	669.65	Joback Method
cpg	326.73	J/molxK	710.47	Joback Method
cpg	336.04	J/molxK	751.29	Joback Method
cpg	344.66	J/molxK	792.12	Joback Method

# Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C23838268&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C23838268&amp;Units=SI</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>rinp:</b>	Non-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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