

# 1-Propene, 1-(ethylthio)-2-methyl-

<b>Inchi:</b>	InChI=1S/C6H12S/c1-4-7-5-6(2)3/h5H,4H2,1-3H3
<b>InchiKey:</b>	WVQJKWZZGMMV DK-UHFFFAOYSA-N
<b>Formula:</b>	C6H12S
<b>SMILES:</b>	CCSC=C(C)C
<b>Mol. weight [g/mol]:</b>	116.22
<b>CAS:</b>	27482-14-0

## Physical Properties

Property code	Value	Unit	Source
gf	104.43	kJ/mol	Joback Method
hf	-17.87	kJ/mol	Joback Method
hfus	14.32	kJ/mol	Joback Method
hvap	35.81	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.663		Crippen Method
mcvol	107.450	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
tb	409.50	K	Joback Method
tc	612.35	K	Joback Method
tf	172.74	K	Joback Method
vc	0.406	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.19	J/mol×K	409.50	Joback Method
cpg	202.53	J/mol×K	443.31	Joback Method
cpg	213.33	J/mol×K	477.12	Joback Method
cpg	223.60	J/mol×K	510.92	Joback Method
cpg	233.36	J/mol×K	544.73	Joback Method
cpg	242.62	J/mol×K	578.54	Joback Method
cpg	251.42	J/mol×K	612.35	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=C27482140&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C27482140&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>

# 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>mccvol:</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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