

# 1-Butene, 1-(ethylthio)-3,3-dimethyl-, (Z)-

Inchi:	InChI=1S/C8H16S/c1-5-9-7-6-8(2,3)4/h6-7H,5H2,1-4H3/b7-6-
InchiKey:	FXSJCQQVGORPDS-SREVYHEPSA-N
Formula:	C8H16S
SMILES:	CCSC=CC(C)(C)C
Mol. weight [g/mol]:	144.28
CAS:	64707-11-5

## Physical Properties

Property code	Value	Unit	Source
gf	132.66	kJ/mol	Joback Method
hf	-58.11	kJ/mol	Joback Method
hfus	13.39	kJ/mol	Joback Method
hvap	38.88	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	3.299		Crippen Method
mcvol	135.630	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
tb	452.15	K	Joback Method
tc	659.90	K	Joback Method
tf	211.66	K	Joback Method
vc	0.506	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.43	J/mol×K	452.15	Joback Method
cpg	288.38	J/mol×K	486.77	Joback Method
cpg	302.45	J/mol×K	521.40	Joback Method
cpg	315.67	J/mol×K	556.02	Joback Method
cpg	328.08	J/mol×K	590.65	Joback Method
cpg	339.75	J/mol×K	625.27	Joback Method
cpg	350.69	J/mol×K	659.90	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=C64707115&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C64707115&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>hvac:</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>mccol:</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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