

# trans-1-(Ethylthio)-2-butene

<b>Inchi:</b>	InChI=1S/C6H12S/c1-3-5-6-7-4-2/h3,5H,4,6H2,1-2H3/b5-3+
<b>InchiKey:</b>	BHFZHOGCQAPTLZ-HWKANZROSA-N
<b>Formula:</b>	C6H12S
<b>SMILES:</b>	CC=CCSCC
<b>Mol. weight [g/mol]:</b>	116.22
<b>CAS:</b>	113664-29-2

## Physical Properties

Property code	Value	Unit	Source
gf	112.98	kJ/mol	Joback Method
hf	-8.08	kJ/mol	Joback Method
hfus	15.63	kJ/mol	Joback Method
hvap	35.73	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	2.316		Crippen Method
mcvol	107.450	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
tb	409.62	K	Joback Method
tc	608.36	K	Joback Method
tf	186.70	K	Joback Method
vc	0.406	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.21	J/mol×K	409.62	Joback Method
cpg	202.37	J/mol×K	442.74	Joback Method
cpg	213.00	J/mol×K	475.87	Joback Method
cpg	223.11	J/mol×K	508.99	Joback Method
cpg	232.74	J/mol×K	542.11	Joback Method
cpg	241.89	J/mol×K	575.24	Joback Method
cpg	250.59	J/mol×K	608.36	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C113664292&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C113664292&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>
<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>

# 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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