

# 1Propene, 1-1'-thiobis-, (Z,Z)-

<b>Inchi:</b>	InChI=1S/C6H10S/c1-3-5-7-6-4-2/h3-6H,1-2H3/b5-3-,6-4-
<b>InchiKey:</b>	RJDJXOBGMMKPMH-GLIMQPGKSA-N
<b>Formula:</b>	C6H10S
<b>SMILES:</b>	CC=CSC=CC
<b>Mol. weight [g/mol]:</b>	114.21
<b>CAS:</b>	37981-36-5

## Physical Properties

Property code	Value	Unit	Source
gf	193.20	kJ/mol	Joback Method
hf	109.14	kJ/mol	Joback Method
hfus	15.83	kJ/mol	Joback Method
hvap	35.68	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.787		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	413.78	K	Joback Method
tc	623.09	K	Joback Method
tf	181.62	K	Joback Method
vc	0.386	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.75	J/molxK	413.78	Joback Method
cpg	186.51	J/molxK	448.66	Joback Method
cpg	196.64	J/molxK	483.55	Joback Method
cpg	206.18	J/molxK	518.43	Joback Method
cpg	215.15	J/molxK	553.32	Joback Method
cpg	223.59	J/molxK	588.20	Joback Method
cpg	231.53	J/molxK	623.09	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=C37981365&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C37981365&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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