

# 2-Propenyl 2,3-bis-(methylthio)propyl ether

**Inchi:** InChI=1S/C8H16OS2/c1-4-5-9-6-8(11-3)7-10-2/h4,8H,1,5-7H2,2-3H3  
**InchiKey:** XVCHWYZDFBUKMR-UHFFFAOYSA-N  
**Formula:** C8H16OS2  
**SMILES:** C=CCOCC(CSC)SC  
**Mol. weight [g/mol]:** 192.34

## Physical Properties

Property code	Value	Unit	Source
gf	63.12	kJ/mol	Joback Method
hf	-136.78	kJ/mol	Joback Method
hfus	21.12	kJ/mol	Joback Method
hvap	48.39	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	2.284		Crippen Method
mcvol	157.850	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
rinpola	1380.00		NIST Webbook
rinpola	1380.00		NIST Webbook
tb	538.66	K	Joback Method
tc	751.59	K	Joback Method
tf	254.19	K	Joback Method
vc	0.585	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.58	J/molxK	538.66	Joback Method
cpg	360.53	J/molxK	574.15	Joback Method
cpg	373.82	J/molxK	609.64	Joback Method
cpg	386.44	J/molxK	645.12	Joback Method
cpg	398.40	J/molxK	680.61	Joback Method
cpg	409.70	J/molxK	716.10	Joback Method
cpg	420.32	J/molxK	751.59	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=R121658&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R121658&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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