

# Episulfide isomer 2

<b>Inchi:</b>	InChI=1S/C5H7NOS/c6-2-1-4(7)5-3-8-5/h4-5,7H,1,3H2
<b>InchiKey:</b>	YHHMEZJFUCZIOV-UHFFFAOYSA-N
<b>Formula:</b>	C5H7NOS
<b>SMILES:</b>	N#CCC(O)C1CS1
<b>Mol. weight [g/mol]:</b>	129.18
<b>CAS:</b>	30381-35-2

## Physical Properties

Property code	Value	Unit	Source
gf	85.75	kJ/mol	Joback Method
hf	-21.10	kJ/mol	Joback Method
hfus	12.57	kJ/mol	Joback Method
hvap	59.22	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	0.376		Crippen Method
mcvol	94.050	ml/mol	McGowan Method
pc	4450.38	kPa	Joback Method
rinpol	1275.70		NIST Webbook
rinpol	1275.70		NIST Webbook
tb	562.19	K	Joback Method
tc	773.12	K	Joback Method
tf	358.31	K	Joback Method
vc	0.357	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.97	J/molxK	562.19	Joback Method
cpg	219.41	J/molxK	597.35	Joback Method
cpg	226.35	J/molxK	632.50	Joback Method
cpg	232.83	J/molxK	667.66	Joback Method
cpg	238.89	J/molxK	702.81	Joback Method
cpg	244.57	J/molxK	737.97	Joback Method
cpg	249.90	J/molxK	773.12	Joback Method

# Sources

<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=C30381352&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C30381352&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>h vap:</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>r in pol:</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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