

# Ethyl neopentyl disulfide

Inchi:	InChI=1S/C7H16S2/c1-5-8-9-6-7(2,3)4/h5-6H2,1-4H3
InchiKey:	GNIXOJWUSQXVCO-UHFFFAOYSA-N
Formula:	C7H16S2
SMILES:	CCSSCC(C)(C)C
Mol. weight [g/mol]:	164.33

## Physical Properties

Property code	Value	Unit	Source
gf	77.14	kJ/mol	Joback Method
hf	-112.82	kJ/mol	Joback Method
hfus	14.73	kJ/mol	Joback Method
hvap	43.51	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.434		Crippen Method
mcvol	142.190	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
rinpol	1141.00		NIST Webbook
ripol	1420.00		NIST Webbook
ripol	1420.00		NIST Webbook
tb	493.89	K	Joback Method
tc	717.04	K	Joback Method
tf	239.87	K	Joback Method
vc	0.524	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.52	J/molxK	493.89	Joback Method
cpg	314.16	J/molxK	531.08	Joback Method
cpg	327.96	J/molxK	568.27	Joback Method
cpg	340.94	J/molxK	605.47	Joback Method
cpg	353.13	J/molxK	642.66	Joback Method
cpg	364.54	J/molxK	679.85	Joback Method
cpg	375.22	J/molxK	717.04	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R602310&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R602310&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>
<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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	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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