

# 2-Diethylaminoethyl vinyl trisulfide

Inchi:	InChI=1S/C8H17NS3/c1-4-9(5-2)7-8-11-12-10-6-3/h6H,3-5,7-8H2,1-2H3
InchiKey:	AAPQWDNLEVLBGA-UHFFFAOYSA-N
Formula:	C8H17NS3
SMILES:	C=CSSSCCN(CC)CC
Mol. weight [g/mol]:	223.42

## Physical Properties

Property code	Value	Unit	Source
gf	314.46	kJ/mol	Joback Method
hf	110.12	kJ/mol	Joback Method
hfus	30.61	kJ/mol	Joback Method
hvap	55.23	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.501		Crippen Method
mcvol	178.310	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
rinpol	1570.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1576.00		NIST Webbook
tb	597.90	K	Joback Method
tc	823.94	K	Joback Method
tf	313.83	K	Joback Method
vc	0.644	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.07	J/molxK	597.90	Joback Method
cpg	423.72	J/molxK	635.57	Joback Method
cpg	437.47	J/molxK	673.25	Joback Method
cpg	450.33	J/molxK	710.92	Joback Method
cpg	462.32	J/molxK	748.59	Joback Method

cpg	473.45	J/mol×K	786.26	Joback Method
cpg	483.75	J/mol×K	823.94	Joback Method

## Sources

<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=R334760&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R334760&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>

## 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>rinpola:</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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