

3-Ethyl-5-vinyl-1,2,4-trithiolane

Other names:	1,2,4-Trithiolane, 5-ethenyl-3-ethyl
Inchi:	InChI=1S/C6H10S3/c1-3-5-7-6(4-2)9-8-5/h3,5-6H,1,4H2,2H3
InchiKey:	NGUCAIBTXVHHKL-UHFFFAOYSA-N
Formula:	C6H10S3
SMILES:	C=CC1SSC(CC)S1
Mol. weight [g/mol]:	178.34

Physical Properties

Property code	Value	Unit	Source
gf	235.90	kJ/mol	Joback Method
hf	134.18	kJ/mol	Joback Method
hfus	15.99	kJ/mol	Joback Method
hvap	45.66	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.363		Crippen Method
mvol	129.290	ml/mol	McGowan Method
pc	3796.32	kPa	Joback Method
rinpol	1366.00		NIST Webbook
tb	487.46	K	Joback Method
tc	737.88	K	Joback Method
tf	412.63	K	Joback Method
vc	0.430	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.25	J/molxK	487.46	Joback Method
cpg	267.05	J/molxK	529.20	Joback Method
cpg	279.90	J/molxK	570.93	Joback Method
cpg	291.86	J/molxK	612.67	Joback Method
cpg	302.98	J/molxK	654.41	Joback Method
cpg	313.30	J/molxK	696.14	Joback Method
cpg	322.89	J/molxK	737.88	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322293&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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