

4-Ethyl-2,3,5-trithiahexane

Other names:	1-(Methylthiopropyl) methyl disulfide Methyl 1-(methylthio)propyl disulphide Disulfide, methyl 1-(methylthio)propyl
Inchi:	InChI=1S/C5H12S3/c1-4-5(6-2)8-7-3/h5H,4H2,1-3H3
InchiKey:	OGKCJWOOFUPRSV-UHFFFAOYSA-N
Formula:	C5H12S3
SMILES:	CCC(SC)SSC
Mol. weight [g/mol]:	168.34
CAS:	53897-66-8

Physical Properties

Property code	Value	Unit	Source
gf	88.14	kJ/mol	Joback Method
hf	-26.20	kJ/mol	Joback Method
hfus	17.57	kJ/mol	Joback Method
hvap	46.79	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	3.097		Crippen Method
mcvol	130.360	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
rinpol	1241.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1265.10		NIST Webbook
rinpol	1220.80		NIST Webbook
rinpol	1265.10		NIST Webbook
tb	519.70	K	Joback Method
tc	763.71	K	Joback Method
tf	234.31	K	Joback Method
vc	0.471	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	258.40	J/mol×K	519.70	Joback Method
cpg	270.44	J/mol×K	560.37	Joback Method
cpg	281.85	J/mol×K	601.04	Joback Method
cpg	292.62	J/mol×K	641.70	Joback Method
cpg	302.74	J/mol×K	682.37	Joback Method
cpg	312.18	J/mol×K	723.04	Joback Method
cpg	320.94	J/mol×K	763.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53897668&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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