Trisulfide, methyl 2-propenyl

Other names:	1-Allyl-3-methyltrisulfane
	Allyl methyl trisulfide
	Allyl methyl trisulphide
	Methyl 2-propenyl trisulfide
	Methyl allyl trisulfide
	Methyl allyl trisulphide
Inchi:	InChI=1S/C4H8S3/c1-3-4-6-7-5-2/h3H,1,4H2,2H3
InchiKey:	JGMPRNFEEAJLAJ-UHFFFAOYSA-N
Formula:	C4H8S3
SMILES:	C=CCSSSC
Mol. weight [g/mol]:	152.30
CAS:	34135-85-8

Physical Properties

Property code	Value	Unit	Source
gf	170.00	kJ/mol	Joback Method
hf	125.15	kJ/mol	Joback Method
hfus	17.23	kJ/mol	Joback Method
hvap	44.28	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.832		Crippen Method
mcvol	111.970	ml/mol	McGowan Method
pc	4391.59	kPa	Joback Method
rinpol	1126.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1123.00		NIST Webbook

rinpol	1142.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1143.80		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1165.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1592.00		NIST Webbook
ripol	1605.00		NIST Webbook
ripol	1591.00		NIST Webbook
ripol	1593.00		NIST Webbook
ripol	1592.00		NIST Webbook
ripol	1593.00		NIST Webbook
ripol	1593.00		NIST Webbook
ripol	1593.00		NIST Webbook
ripol	1588.00		NIST Webbook
tb	493.94	K	Joback Method
tc	742.75	K	Joback Method
tf	236.28	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.51	J/mol×K	493.94	Joback Method
cpg	208.84	J/mol×K	535.41	Joback Method
cpg	217.68	J/mol×K	576.88	Joback Method
cpg	226.02	J/mol×K	618.34	Joback Method
cpg	233.84	J/mol×K	659.81	Joback Method
cpg	241.13	J/mol×K	701.28	Joback Method
cpg	247.89	J/mol×K	742.75	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34135858&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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