methyl trans-1-propenyl trisulfide

Other names: Methyl 1-propenyl trisulfide, (E)-
Methyl 1-propenyl trisulphide, trans
Trisulfide, methyl-1-propenyl, (E)-
Trisulfide, methyl-(E)-1-propenyl
Inchi: InChI=1S/C4H8S3/c1-3-4-6-7-5-2/h3-4H,1-2H3/b4-3+
InchiKey: WPRUFZZPIFLBDG-ONEGZZNKSA-N
Formula: C4H8S3
SMILES: CC=CSSSC
Mol. weight [g/mol]: 152.30

Physical Properties

Property code	Value	Unit	Source
gf	162.38	kJ/mol	Joback Method
hf	116.94	kJ/mol	Joback Method
hfus	18.71	kJ/mol	Joback Method
hvap	44.91	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.179		Crippen Method
mcvol	111.970	ml/mol	McGowan Method
pc	4450.38	kPa	Joback Method
rinpol	1144.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1130.60		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1146.00		NIST Webbook
tb	501.42	K	Joback Method
tc	756.84	K	Joback Method
tf	232.96	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.58	J/mol×K	501.42	Joback Method
cpg	208.10	J/mol×K	543.99	Joback Method
cpg	217.06	J/mol×K	586.56	Joback Method
cpg	225.46	J/mol×K	629.13	Joback Method
cpg	233.29	J/mol×K	671.70	Joback Method
cpg	240.57	J/mol×K	714.27	Joback Method
cpg	247.28	J/mol×K	756.84	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R53383&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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