3-Methyl-1,2,4-trithiane

Other names: 1,2,4-Trithiane, 3-methyl
Inchi: InChI=1S/C4H8S3/c1-4-5-2-3-6-7-4/h4H,2-3H2,1H3
InchiKey: UXPUEXDAOSQIQS-UHFFFAOYSA-N
Formula: C4H8S3
SMILES: CC1SCCSS1
Mol. weight [g/mol]: 152.30

Physical Properties

Property code	Value	Unit	Source
gf	126.83	kJ/mol	Joback Method
hf	64.21	kJ/mol	Joback Method
hfus	8.92	kJ/mol	Joback Method
hvap	42.36	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.461		Crippen Method
mcvol	105.410	ml/mol	McGowan Method
pc	4994.44	kPa	Joback Method
rinpol	1243.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1266.00		NIST Webbook
ripol	1852.00		NIST Webbook
ripol	1862.00		NIST Webbook
tb	453.96	K	Joback Method
tc	718.89	K	Joback Method
tf	392.57	K	Joback Method
vc	0.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.98	J/mol×K	453.96	Joback Method
cpg	199.50	J/mol×K	498.11	Joback Method
cpg	211.14	J/mol×K	542.27	Joback Method
cpg	221.95	J/mol×K	586.42	Joback Method
cpg	231.97	J/mol×K	630.58	Joback Method
cpg	241.23	J/mol×K	674.73	Joback Method
cpg	249.78	J/mol×K	718.89	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=C43040013&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