4,6-Dimethyl-[1,2,3]trithiane

Other names: 3,5-dimethyl-1,2,6-trithiane
Inchi: InChI=1S/C5H10S3/c1-4-3-5(2)7-8-6-4/h4-5H,3H2,1-2H3
InchiKey: JJKQDZKSTXTCRP-UHFFFAOYSA-N
Formula: C5H10S3
SMILES: CC1CC(C)SSS1
Mol. weight [g/mol]: 166.33

Physical Properties

Property code	Value	Unit	Source
gf	127.54	kJ/mol	Joback Method
hf	23.23	kJ/mol	Joback Method
hfus	12.58	kJ/mol	Joback Method
hvap	44.28	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.197		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
rinpol	1265.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1265.00		NIST Webbook
tb	472.17	K	Joback Method
tc	731.77	K	Joback Method
tf	399.60	K	Joback Method
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.14	J/mol×K	472.17	Joback Method
cpg	242.55	J/mol×K	515.44	Joback Method
cpg	256.04	J/mol×K	558.70	Joback Method
cpg	268.65	J/mol×K	601.97	Joback Method

cpg	280.41	J/mol×K	645.24	Joback Method
cpg	291.33	J/mol×K	688.50	Joback Method
cpg	301.46	J/mol×K	731.77	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U186039&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
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