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]: 166.34

Physical Properties

Property code	Value	Unit	Source
hfus	12.58	kJ/mol	Joback Method
logp	3.197		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
rinpol	1265.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1265.00		NIST Webbook

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U186039&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices