

4,6-dimethyl-1,2,3,5-tetrathiane

Other names:	1,2,3,5-Tetrathiane, 4,6-dimethyl 4,6-dimethyl-1,2,3,5-tetrathiacyclohexane
Inchi:	InChI=1S/C4H8S4/c1-3-5-4(2)7-8-6-3/h3-4H,1-2H3
InchiKey:	LIAYFMNHMJEGEI-UHFFFAOYSA-N
Formula:	C4H8S4
SMILES:	CC1SSSC(C)S1
Mol. weight [g/mol]:	184.37

Physical Properties

Property code	Value	Unit	Source
gf	158.98	kJ/mol	Joback Method
hf	89.13	kJ/mol	Joback Method
hfus	13.65	kJ/mol	Joback Method
hvap	47.87	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.455		Crippen Method
mcvol	121.760	ml/mol	McGowan Method
pc	4730.11	kPa	Joback Method
rinpol	1390.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1389.00		NIST Webbook
ripol	2016.00		NIST Webbook
ripol	2016.00		NIST Webbook
ripol	2061.00		NIST Webbook
tb	497.12	K	Joback Method
tc	778.61	K	Joback Method
tf	471.78	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.67	J/mol×K	497.12	Joback Method

cpg	240.52	J/mol×K	544.04	Joback Method
cpg	252.45	J/mol×K	590.95	Joback Method
cpg	263.51	J/mol×K	637.87	Joback Method
cpg	273.71	J/mol×K	684.78	Joback Method
cpg	283.10	J/mol×K	731.70	Joback Method
cpg	291.71	J/mol×K	778.61	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=R44576&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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