4,6-dimethyl-1,2,5-trithiepane

Other names: 1,2,5-Trithiepane, 4,6-dimethyl
Inchi: InChI=1S/C6H12S3/c1-5-3-7-8-4-6(2)9-5/h5-6H,3-4H2,1-2H3
InchiKey: NALUNDQPIYLHAN-UHFFFAOYSA-N
Formula: C6H12S3
SMILES: CC1CSSCC(C)S1
Mol. weight [g/mol]: 180.35

Physical Properties

Property code	Value	Unit	Source
gf	123.86	kJ/mol	Joback Method
hf	-3.57	kJ/mol	Joback Method
hfus	13.07	kJ/mol	Joback Method
hvap	46.68	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.892		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
rinpol	1442.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1454.00		NIST Webbook
tb	499.32	K	Joback Method
tc	764.15	K	Joback Method
tf	407.35	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.66	J/mol×K	499.32	Joback Method
cpg	286.52	J/mol×K	543.46	Joback Method
cpg	302.30	J/mol×K	587.60	Joback Method
cpg	317.02	J/mol×K	631.74	Joback Method
cpg	330.71	J/mol×K	675.88	Joback Method
cpg	343.38	J/mol×K	720.01	Joback Method

cpg	355.05	J/mol×K	764.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R82320&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