1,2,4,6-Tetrathiepane, 3,5,7-trimethyl, #1

Inchi: InChI=1S/C6H12S4/c1-4-7-5(2)9-10-6(3)8-4/h4-6H,1-3H3
InchiKey: WMWRKEXBIGLGBW-UHFFFAOYSA-N
Formula: C6H12S4
SMILES: CC1SSC(C)SC(C)S1
Mol. weight [g/mol]: 212.42

Physical Properties

Property code	Value	Unit	Source
gf	156.01	kJ/mol	Joback Method
hf	21.35	kJ/mol	Joback Method
hfus	17.80	kJ/mol	Joback Method
hvap	52.18	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.886		Crippen Method
mcvol	149.940	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
rinpol	1511.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1526.00		NIST Webbook
tb	542.48	K	Joback Method
tc	821.95	K	Joback Method
tf	486.56	K	Joback Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.07	J/mol×K	542.48	Joback Method
cpg	332.22	J/mol×K	589.06	Joback Method
cpg	348.20	J/mol×K	635.64	Joback Method
cpg	363.03	J/mol×K	682.22	Joback Method
cpg	376.73	J/mol×K	728.79	Joback Method
cpg	389.29	J/mol×K	775.37	Joback Method
cpg	400.73	J/mol×K	821.95	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=R44601&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume