5,6-dimethyl-2,3,7-trithiabicyclo[2.2.1] heptane

Inchi: InChI=1S/C6H10S3/c1-3-4(2)6-7-5(3)8-9-6/h3-6H,1-2H3
InchiKey: VPUSWHBKDZKTGL-UHFFFAOYSA-N
Formula: C6H10S3
SMILES: CC1C2SSC(S2)C1C
Mol. weight [g/mol]: 178.34

Physical Properties

Property code	Value	Unit	Source
gf	213.20	kJ/mol	Joback Method
hf	67.37	kJ/mol	Joback Method
hfus	18.58	kJ/mol	Joback Method
hvap	45.77	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.053		Crippen Method
mcvol	122.730	ml/mol	McGowan Method
pc	3940.66	kPa	Joback Method
rinpol	1346.00		NIST Webbook
rinpol	1346.00		NIST Webbook
tb	488.58	K	Joback Method
tc	743.69	K	Joback Method
tf	431.61	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.50	J/mol×K	488.58	Joback Method
cpg	272.67	J/mol×K	531.10	Joback Method
cpg	286.67	J/mol×K	573.62	Joback Method
cpg	299.59	J/mol×K	616.14	Joback Method
cpg	311.52	J/mol×K	658.65	Joback Method
cpg	322.54	J/mol×K	701.17	Joback Method
cpg	332.76	J/mol×K	743.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R56866&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