1,2,3,5-Trithiazine, perhydro, 4,6-dimethyl

Inchi: InChI=1S/C4H9NS3/c1-3-5-4(2)7-8-6-3/h3-5H,1-2H3
InchiKey: BOGSLBMMIZYSFR-UHFFFAOYSA-N
Formula: C4H9NS3
SMILES: CC1NC(C)SSS1
Mol. weight [g/mol]: 167.32

Physical Properties

Property code	Value	Unit	Source
gf	206.83	kJ/mol	Joback Method
hf	81.68	kJ/mol	Joback Method
hfus	19.58	kJ/mol	Joback Method
hvap	48.81	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.311		Crippen Method
mcvol	115.390	ml/mol	McGowan Method
pc	4938.44	kPa	Joback Method
rinpol	1110.00		NIST Webbook
rinpol	1110.00		NIST Webbook
tb	497.84	K	Joback Method
tc	768.60	K	Joback Method
tf	493.36	K	Joback Method
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.64	J/mol×K	497.84	Joback Method
cpg	236.94	J/mol×K	542.97	Joback Method
cpg	249.44	J/mol×K	588.09	Joback Method
cpg	261.15	J/mol×K	633.22	Joback Method
cpg	272.07	J/mol×K	678.35	Joback Method
cpg	282.21	J/mol×K	723.48	Joback Method
cpg	291.57	J/mol×K	768.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R44651&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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