1,3,5-Oxathiazine, perhydro, 2,4,6-trimethyl

Inchi: InChI=1S/C6H13NOS/c1-4-7-5(2)9-6(3)8-4/h4-7H,1-3H3
InchiKey: HINMBHROYKGEJD-UHFFFAOYSA-N
Formula: C6H13NOS
SMILES: CC1NC(C)SC(C)O1
Mol. weight [g/mol]: 147.24

Physical Properties

Property code	Value	Unit	Source
gf	50.12	kJ/mol	Joback Method
hf	-202.46	kJ/mol	Joback Method
hfus	26.50	kJ/mol	Joback Method
hvap	45.84	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	1.377		Crippen Method
mcvol	116.740	ml/mol	McGowan Method
pc	3695.46	kPa	Joback Method
rinpol	992.00		NIST Webbook
tb	470.22	K	Joback Method
tc	698.44	K	Joback Method
tf	371.33	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.17	J/mol×K	470.22	Joback Method
cpg	266.94	J/mol×K	508.26	Joback Method
cpg	282.00	J/mol×K	546.29	Joback Method
cpg	296.35	J/mol×K	584.33	Joback Method
cpg	309.96	J/mol×K	622.37	Joback Method
cpg	322.84	J/mol×K	660.41	Joback Method
cpg	334.98	J/mol×K	698.44	Joback Method

Sources

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=R44718&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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