4,6-dimethyl-2-(propan-2-yl)-1,3,5-dithiazinane

Other names: 1,3,5-Dithiazine, perhydro-4,6-dimethyl-2-(1-methylethyl)
Inchi: InChI=1S/C8H17NS2/c1-5(2)8-10-6(3)9-7(4)11-8/h5-9H,1-4H3
InchiKey: ZNOHVVXGIQIPAU-UHFFFAOYSA-N
Formula: C8H17NS2
SMILES: CC1NC(C)SC(C(C)C)S1
Mol. weight [g/mol]: 191.36
CAS: 104691-40-9

Physical Properties

Property code	Value	Unit	Source
gf	190.50	kJ/mol	Joback Method
hf	-71.76	kJ/mol	Joback Method
hfus	23.83	kJ/mol	Joback Method
hvap	51.21	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.730		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
tb	536.42	K	Joback Method
tc	777.58	K	Joback Method
tf	435.75	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.29	J/mol×K	536.42	Joback Method
cpg	377.25	J/mol×K	576.61	Joback Method
cpg	395.16	J/mol×K	616.81	Joback Method
cpg	412.03	J/mol×K	657.00	Joback Method
cpg	427.87	J/mol×K	697.19	Joback Method
cpg	442.68	J/mol×K	737.39	Joback Method
cpg	456.48	J/mol×K	777.58	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104691409&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume