1,3,5-Dithiazine, perhydro, 4,6-dimethyl-2-(2-methylpropyl)

Inchi: InChI=1S/C9H19NS2/c1-6(2)5-9-11-7(3)10-8(4)12-9/h6-10H,5H2,1-4H3
InchiKey: FVPPILNIVWRBNY-UHFFFAOYSA-N
Formula: C9H19NS2
SMILES: CC(C)CC1SC(C)NC(C)S1
Mol. weight [g/mol]: 205.38

Physical Properties

Property code	Value	Unit	Source
gf	198.92	kJ/mol	Joback Method
hf	-92.40	kJ/mol	Joback Method
hfus	26.42	kJ/mol	Joback Method
hvap	53.43	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.120		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	1423.00		NIST Webbook
rinpol	1423.00		NIST Webbook
tb	559.30	K	Joback Method
tc	795.63	K	Joback Method
tf	447.02	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.50	J/mol×K	559.30	Joback Method
cpg	426.24	J/mol×K	598.69	Joback Method
cpg	444.87	J/mol×K	638.08	Joback Method
cpg	462.40	J/mol×K	677.46	Joback Method
cpg	478.86	J/mol×K	716.85	Joback Method
cpg	494.25	J/mol×K	756.24	Joback Method
cpg	508.58	J/mol×K	795.63	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=R62261&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