1,3,5-Dithiazine, perhydro-6-butyl-2,4-dimethyl

Inchi: InChI=1S/C9H19NS2/c1-4-5-6-9-10-7(2)11-8(3)12-9/h7-10H,4-6H2,1-3H3
InchiKey: ZGCDSMJNRUXZGG-UHFFFAOYSA-N
Formula: C9H19NS2
SMILES: CCCCC1NC(C)SC(C)S1
Mol. weight [g/mol]: 205.38

Physical Properties

Property code	Value	Unit	Source
gf	201.36	kJ/mol	Joback Method
hf	-87.12	kJ/mol	Joback Method
hfus	29.95	kJ/mol	Joback Method
hvap	53.82	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.264		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	1415.00		NIST Webbook
rinpol	1415.00		NIST Webbook
tb	559.74	K	Joback Method
tc	790.77	K	Joback Method
tf	462.02	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.18	J/mol×K	559.74	Joback Method
cpg	425.41	J/mol×K	598.25	Joback Method
cpg	443.60	J/mol×K	636.75	Joback Method
cpg	460.75	J/mol×K	675.26	Joback Method
cpg	476.88	J/mol×K	713.76	Joback Method
cpg	492.00	J/mol×K	752.27	Joback Method
cpg	506.12	J/mol×K	790.77	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=R62289&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