1,3,5-Dithiazine, perhydro, 2,4,6-trimethyl, #3

Inchi: InChI=1S/C6H13NS2/c1-4-7-5(2)9-6(3)8-4/h4-7H,1-3H3
InchiKey: FBMVFHKKLDGLJA-UHFFFAOYSA-N
Formula: C6H13NS2
SMILES: CC1NC(C)SC(C)S1
Mol. weight [g/mol]: 163.30

Physical Properties

Property code	Value	Unit	Source
gf	176.10	kJ/mol	Joback Method
hf	-25.20	kJ/mol	Joback Method
hfus	22.18	kJ/mol	Joback Method
hvap	47.14	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.094		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
rinpol	1211.00		NIST Webbook
rinpol	1211.00		NIST Webbook
tb	491.10	K	Joback Method
tc	736.07	K	Joback Method
tf	428.21	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.18	J/mol×K	491.10	Joback Method
cpg	283.57	J/mol×K	531.93	Joback Method
cpg	299.12	J/mol×K	572.76	Joback Method
cpg	313.83	J/mol×K	613.58	Joback Method
cpg	327.70	J/mol×K	654.41	Joback Method
cpg	340.72	J/mol×K	695.24	Joback Method
cpg	352.89	J/mol×K	736.07	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=R44697&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