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

Other names: 1,3,5-Dithiazine, perhydro, 2,4,6-trimethyl, #2
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]: 163.31

Physical Properties

Property code	Value	Unit	Source
hfus	22.18	kJ/mol	Joback Method
ie	8.29	eV	Cheméo Relay (1.0)
logp	2.094		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
rinpol	1204.00		NIST Webbook
rinpol	1204.00		NIST Webbook

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R44683&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices