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

Inchi: InChI=1S/C6H14N2S/c1-4-7-5(2)9-6(3)8-4/h4-8H,1-3H3
InchiKey: PLCVUJTXVJDGBN-UHFFFAOYSA-N
Formula: C6H14N2S
SMILES: CC1NC(C)SC(C)N1
Mol. weight [g/mol]: 146.25

Physical Properties

Property code	Value	Unit	Source
gf	223.95	kJ/mol	Joback Method
hf	-32.65	kJ/mol	Joback Method
hfus	28.11	kJ/mol	Joback Method
hvap	48.09	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	0.950		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
rinpol	1056.00		NIST Webbook
rinpol	1056.00		NIST Webbook
tb	491.82	K	Joback Method
tc	727.92	K	Joback Method
tf	449.79	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.12	J/mol×K	491.82	Joback Method
cpg	279.73	J/mol×K	531.17	Joback Method
cpg	295.59	J/mol×K	570.52	Joback Method
cpg	310.70	J/mol×K	609.87	Joback Method
cpg	325.04	J/mol×K	649.22	Joback Method
cpg	338.58	J/mol×K	688.57	Joback Method
cpg	351.32	J/mol×K	727.92	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=R44722&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

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