

3,4,5,6-Tetrahydro-2,4,6-trimethyl-2H-1,3,5-thiadiazine

Other names:	1,3,5-Thiadiazine, perhydro-2,4,6-trimethyl 2,4,6-Trimethyltetrahydro-1,3,5-thiadiazine
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
CAS:	53897-63-5

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
mvol	120.850	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
rinpol	1066.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1062.00		NIST Webbook
tb	491.82	K	Joback Method
tc	727.92	K	Joback Method
tf	449.79	K	Joback Method
vc	0.422	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.12	J/molxK	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53897635&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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