5,6-Dihydro-2,4,6-trimethyl-4H-1,3,5-dithiazine

Other names:	2,4,6-trimethylperhydro-1,3,5-dithiazine thialdine 1,3,5-Dithiazine, perhydro-2,4,6-trimethyl 2,4,6-trimethyl-1,3,5-dithiazine (thialdine) 5,6-Dihydro-2,4,6-trimethyl-1,3,5-dithiazine (thialdine) Dihydro-2,4,6-trimethyl-1,3,5(4H)-dithiazine (thialdine) thialdin 2,4,6-trimethyldihydro-1,3,5-dithiazine (thialdine) 5,6-dihydro-2,4,6-trimethyl-1,3,5-dithiazine
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
CAS:	638-17-5

Physical Properties

Property code	Value	Unit	Source
chs	-5286.90	kJ/mol	NIST Webbook
gf	176.10	kJ/mol	Joback Method
hf	-25.20	kJ/mol	Joback Method
hfs	-138.00	kJ/mol	NIST Webbook
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	1150.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1202.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1166.90		NIST Webbook
rinpol	1168.00		NIST Webbook
ripol	1750.00		NIST Webbook

ripol	1756.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1786.00		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

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=C638175&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase 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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume