

2H-1,3,4-Thiadiazine, tetrahydro-2,2-dimethyl-

Inchi:	InChI=1S/C5H12N2S/c1-5(2)7-6-3-4-8-5/h6-7H,3-4H2,1-2H3
InchiKey:	ZZOFOVXIYBTNMZ-UHFFFAOYSA-N
Formula:	C5H12N2S
SMILES:	CC1(C)NNCCS1
Mol. weight [g/mol]:	132.23
CAS:	69247-72-9

Physical Properties

Property code	Value	Unit	Source
gf	225.46	kJ/mol	Joback Method
hf	43.91	kJ/mol	Joback Method
hfus	17.08	kJ/mol	Joback Method
hvap	45.33	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	0.564		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	5073.01	kPa	Joback Method
tb	478.52	K	Joback Method
tc	730.52	K	Joback Method
tf	470.90	K	Joback Method
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.61	J/molxK	478.52	Joback Method
cpg	233.13	J/molxK	520.52	Joback Method
cpg	246.62	J/molxK	562.52	Joback Method
cpg	259.21	J/molxK	604.52	Joback Method
cpg	271.03	J/molxK	646.52	Joback Method
cpg	282.22	J/molxK	688.52	Joback Method
cpg	292.91	J/molxK	730.52	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69247729&Units=SI

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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