

# 1,2,4,5-Tetrazine, hexahydro-1,2,4,5-tetramethyl-

**Other names:** 1,2,4,5-Tetramethyl-1,2,4,5-tetraazinane  
1,2,4,5-Tetraazacyclohexane, 1,2,4,5-tetramethyl-  
s-Tetrazine, hexahydro-1,2,4,5-tetramethyl-

**Inchi:** InChI=1S/C6H16N4/c1-7-5-9(3)10(4)6-8(7)2/h5-6H2,1-4H3

**InchiKey:** FTQDWTRRRXIFSL-UHFFFAOYSA-N

**Formula:** C6H16N4

**SMILES:** CN1CN(C)N(C)CN1C

**Mol. weight [g/mol]:** 144.22

**CAS:** 20717-38-8

## Physical Properties

Property code	Value	Unit	Source
ie	6.84 ± 0.05	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
log10ws	0.52		Crippen Method
logp	-0.528		Crippen Method
mvol	124.460	ml/mol	McGowan Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C20717388&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**ie:** Ionization energy  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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