

1,2,4,5-Tetrazine, 3,6-dimethyl-

Other names:	s-Tetrazine, 3,6-dimethyl- Dimethyl-s-tetrazine
Inchi:	InChI=1S/C4H6N4/c1-3-5-7-4(2)8-6-3/h1-2H3
InchiKey:	DGLYTMLIGRQDPE-UHFFFAOYSA-N
Formula:	C4H6N4
SMILES:	Cc1nnc(C)nn1
Mol. weight [g/mol]:	110.12
CAS:	1558-23-2

Physical Properties

Property code	Value	Unit	Source
ie	9.08	eV	NIST Webbook
log10ws	-1.49		Crippen Method
logp	-0.117		Crippen Method
mcvol	83.380	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1558232&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	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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