

1,3,5-Triazine, 1,3,5-triethylhexahydro-

Other names:	s-Triazine, 1,3,5-triethylhexahydro- Hexahydro-1,3,5-triethyl-s-triazine Triethyltrimethylenetriamine Vancide TH 1,3,5-Triethylhexahydro-s-triazine 1,3,5-Triethylhexahydro-1,3,5-triazine 1,3,5-Triethylhexahydro-sym-triazine s-Triazine, hexahydro-1,3,5-triethyl- hexahydro-1,3,5-triethyl-1,3,5-triazine
Inchi:	InChI=1S/C9H21N3/c1-4-10-7-11(5-2)9-12(6-3)8-10/h4-9H2,1-3H3
InchiKey:	XYRTVIAPRQLSOW-UHFFFAOYSA-N
Formula:	C9H21N3
SMILES:	CCN1CN(CC)CN(CC)C1
Mol. weight [g/mol]:	171.28
CAS:	7779-27-3

Physical Properties

Property code	Value	Unit	Source
ie	7.40	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-0.68		Crippen Method
logp	0.838		Crippen Method
mcvol	156.750	ml/mol	McGowan Method
tb	480.70	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7779273&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
tb:	Normal Boiling Point Temperature

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