

# 1,3,5-Triazine, hexahydro-1,3,5-tris(1-methylethyl)-

Other names:	s-Triazine, hexahydro-1,3,5-triisopropyl- Hexahydro-1,3,5-triisopropyl-s-triazine 1,3,5-Triisopropylhexahydro-1,3,5-triazine 1,3,5-Triisopropyl hexahydro-sym-triazine
Inchi:	InChI=1S/C12H27N3/c1-10(2)13-7-14(11(3)4)9-15(8-13)12(5)6/h10-12H,7-9H2,1-6H3
InchiKey:	FBXRCTMIDHCRDT-UHFFFAOYSA-N
Formula:	C12H27N3
SMILES:	CC(C)N1CN(C(C)C)CN(C(C)C)C1
Mol. weight [g/mol]:	213.36
CAS:	10556-98-6

## Physical Properties

Property code	Value	Unit	Source
ie	7.50	eV	NIST Webbook
ie	7.95	eV	NIST Webbook
log10ws	-2.27		Crippen Method
logp	2.004		Crippen Method
mcvol	199.020	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C10556986&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10556986&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## 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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