

1,3,5-Triazine, hexahydro-1,3,5-triphenyl-

Other names:	s-Triazine, hexahydro-1,3,5-triphenyl- Anhydroformaldehyde aniline 1,3,5-Triphenylhexahydro-s-triazine 1,3,5-Triphenylhexahydro-1,3,5-triazine Hexahydro-1,3,5-triphenyl-1,3,5-triazine Methyleneaniline trimer 1,3,5-Triphenylhexahydrotriazine Hexahydro-1,3,5-triphenyl-S-triazine
Inchi:	InChI=1S/C21H21N3/c1-4-10-19(11-5-1)22-16-23(20-12-6-2-7-13-20)18-24(17-22)21-14
InchiKey:	VASMRQAVWVVDPA-UHFFFAOYSA-N
Formula:	C ₂₁ H ₂₁ N ₃
SMILES:	<chem>c1ccc(N2CN(c3ccccc3)CN(c3ccccc3)C2)cc1</chem>
Mol. weight [g/mol]:	315.41
CAS:	91-78-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.62		Crippen Method
logp	4.392		Crippen Method
mcvol	254.550	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91781&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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