

# 6-Chloro-N,N'-(1,3,3-trimethylbutyl)-[1,3,5]triazine-

**Inchi:** InChI=1S/C17H32ClN5/c1-11(9-16(3,4)5)19-14-21-13(18)22-15(23-14)20-12(2)10-17(6,7)  
**InchiKey:** MFORFBJBHLBNSR-UHFFFAOYSA-N  
**Formula:** C17H32ClN5  
**SMILES:** CC(CC(C)(C)C)Nc1nc(Cl)nc(NC(C)CC(C)(C)C)n1  
**Mol. weight [g/mol]:** 341.92

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.24		Crippen Method
logp	4.998		Crippen Method
mcpvol	288.770	ml/mol	McGowan Method
rinpol	2235.62		NIST Webbook
rinpol	2251.95		NIST Webbook
rinpol	2235.62		NIST Webbook
rinpol	2255.14		NIST Webbook
rinpol	2271.67		NIST Webbook
rinpol	2251.95		NIST Webbook
rinpol	2271.48		NIST Webbook
rinpol	2235.62		NIST Webbook
rinpol	2251.95		NIST Webbook

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R288632&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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