

# 6-Chloro-N,N'-(1,1,3,3-tetramethylbutyl)-[1,3,5]triazole

**Inchi:** InChI=1S/C19H36ClN5/c1-16(2,3)11-18(7,8)24-14-21-13(20)22-15(23-14)25-19(9,10)12-18  
**InchiKey:** NFQMVGPFOLFABQN-UHFFFAOYSA-N  
**Formula:** C19H36ClN5  
**SMILES:** CC(C)(C)CC(C)(C)Nc1nc(Cl)nc(NC(C)(C)CC(C)(C)C)n1  
**Mol. weight [g/mol]:** 369.98

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -7.07   |        | Crippen Method |
| logp          | 5.778   |        | Crippen Method |
| mccvol        | 316.950 | ml/mol | McGowan Method |
| rinpol        | 2344.28 |        | NIST Webbook   |
| rinpol        | 2390.01 |        | NIST Webbook   |
| rinpol        | 2344.28 |        | NIST Webbook   |
| rinpol        | 2363.13 |        | NIST Webbook   |
| rinpol        | 2373.88 |        | NIST Webbook   |
| rinpol        | 2390.01 |        | NIST Webbook   |
| rinpol        | 2408.88 |        | NIST Webbook   |
| rinpol        | 2344.28 |        | NIST Webbook   |
| rinpol        | 2390.01 |        | NIST Webbook   |

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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=R288578&Units=SI>

## Legend

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

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

Latest version available from:

<https://www.cheméo.com/cid/66-373-5/6-Chloro-N-N-1-1-3-3-tetramethylbutyl-1-3-5-triazine-2-4-diamine.pdf>

Generated by Cheméo on 2024-04-26 21:59:51.129718862 +0000 UTC m=+16458040.050296194.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.