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

**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-
**InchiKey:** NFQMVGPOLFABQN-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 |
| mcvol | 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/ci990307l
**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=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