

# 6-Chloro-N,N'-(cyclobutyl)-[1,3,5]triazine-2,4-diam

**Inchi:** InChI=1S/C11H16ClN5/c12-9-15-10(13-7-3-1-4-7)17-11(16-9)14-8-5-2-6-8/h7-8H,1-6H2,  
**InchiKey:** WGWFUVPOZDRVAO-UHFFFAOYSA-N  
**Formula:** C11H16ClN5  
**SMILES:** Clc1nc(=NC2CCC2)[nH]c(=NC2CCC2)[nH]1  
**Mol. weight [g/mol]:** 253.73

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.21		Crippen Method
logp	0.334		Crippen Method
mcvol	182.510	ml/mol	McGowan Method
rinpol	2146.08		NIST Webbook
rinpol	2146.08		NIST Webbook
rinpol	2192.25		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=R288414&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

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