

# (4,6-Dichloro-[1,3,5]triazin-2-yl)-(1,1-dimethyl-propyl)amine

**Inchi:** InChI=1S/C8H12Cl2N4/c1-4-8(2,3)14-7-12-5(9)11-6(10)13-7/h4H2,1-3H3,(H,11,12,13,14)  
**InchiKey:** HIIWTFPAKHZRAW-UHFFFAOYSA-N  
**Formula:** C8H12Cl2N4  
**SMILES:** CCC(C)(C)Nc1nc(Cl)nc(Cl)n1  
**Mol. weight [g/mol]:** 235.11

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	2.779		Crippen Method
mcpvol	164.220	ml/mol	McGowan Method
rinpol	1617.49		NIST Webbook
rinpol	1647.65		NIST Webbook
rinpol	1617.49		NIST Webbook
rinpol	1625.39		NIST Webbook
rinpol	1637.68		NIST Webbook
rinpol	1647.65		NIST Webbook
rinpol	1655.57		NIST Webbook
rinpol	1617.49		NIST Webbook
rinpol	1647.65		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=R288543&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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