

# (4,6-Dichloro-[1,3,5]triazin-2-yl)-(1-methyl-butyl)-a

**Inchi:** InChI=1S/C8H12Cl2N4/c1-3-4-5(2)11-8-13-6(9)12-7(10)14-8/h5H,3-4H2,1-2H3,(H,11,12,  
**InchiKey:** RBJAOUBQAQYPIF-UHFFFAOYSA-N  
**Formula:** C8H12Cl2N4  
**SMILES:** CCCC(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
mcpol	164.220	ml/mol	McGowan Method
rinpol	1643.16		NIST Webbook
rinpol	1668.31		NIST Webbook
rinpol	1643.16		NIST Webbook
rinpol	1670.78		NIST Webbook
rinpol	1668.31		NIST Webbook
rinpol	1678.79		NIST Webbook
rinpol	1643.16		NIST Webbook
rinpol	1668.31		NIST Webbook
rinpol	1653.61		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R288563&Units=SI>  
**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)

## 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/124-710-5/4-6-Dichloro-1-3-5-triazin-2-yl-1-methyl-butyl-amine.pdf>

Generated by Cheméo on 2024-04-27 23:20:55.838951559 +0000 UTC m=+16549304.759528870.

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