

6-Chloro-N,N'-(cyclohexyl)-[1,3,5]triazine-2,4-diamine

Inchi: InChI=1S/C15H24ClN5/c16-13-19-14(17-11-7-3-1-4-8-11)21-15(20-13)18-12-9-5-2-6-10-1
InchiKey: YHVSDOGDOJTVJQ-UHFFFAOYSA-N
Formula: C15H24ClN5
SMILES: Clc1nc(=NC2CCCCC2)[nH]c(=NC2CCCCC2)[nH]1
Mol. weight [g/mol]: 309.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.88		Crippen Method
logp	1.894		Crippen Method
mcvol	238.870	ml/mol	McGowan Method
rinpol	2345.05		NIST Webbook
rinpol	2391.99		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R288454&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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

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