

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

Inchi: InChI=1S/C9H12ClN5/c10-7-13-8(11-5-1-2-5)15-9(14-7)12-6-3-4-6/h5-6H,1-4H2,(H2,11,12,13,14,15)N
InchiKey: JOLQRGPIGYOFHI-UHFFFAOYSA-N
Formula: C9H12ClN5
SMILES: Clc1nc(NC2CC2)nc(NC2CC2)n1
Mol. weight [g/mol]: 225.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	1.674		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
rinpole	2048.58		NIST Webbook
rinpole	2086.66		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R288494&Units=SI>
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>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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