

6-Chloro-N,N'-(1,2-dimethylpropyl)-[1,3,5]triazine-

Inchi: InChI=1S/C13H24ClN5/c1-7(2)9(5)15-12-17-11(14)18-13(19-12)16-10(6)8(3)4/h7-10H,1-
InchiKey: NMYHEKLZENFZLL-UHFFFAOYSA-N
Formula: C13H24ClN5
SMILES: CC(C)C(C)Nc1nc(Cl)nc(NC(C)C(C)C)n1
Mol. weight [g/mol]: 285.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.56		Crippen Method
logp	3.438		Crippen Method
mcpvol	232.410	ml/mol	McGowan Method
rinpol	2032.28		NIST Webbook
rinpol	2055.34		NIST Webbook
rinpol	2032.28		NIST Webbook
rinpol	2043.05		NIST Webbook
rinpol	2061.13		NIST Webbook
rinpol	2055.34		NIST Webbook
rinpol	2066.14		NIST Webbook
rinpol	2032.28		NIST Webbook
rinpol	2055.34		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: 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=R288627&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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