

6-Chloro-N,N'-(1,2,2-trimethylpropyl)-[1,3,5]triazin

Inchi: InChI=1S/C15H28ClN5/c1-9(14(3,4)5)17-12-19-11(16)20-13(21-12)18-10(2)15(6,7)8/h9-
InchiKey: BOQLVHUWEAJSNS-UHFFFAOYSA-N
Formula: C15H28ClN5
SMILES: CC(Nc1nc(Cl)nc(NC(C)C(C)(C)C)n1)C(C)(C)C
Mol. weight [g/mol]: 313.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Crippen Method
logp	4.218		Crippen Method
mcvol	260.590	ml/mol	McGowan Method
rinpol	2122.01		NIST Webbook
rinpol	2146.94		NIST Webbook
rinpol	2122.01		NIST Webbook
rinpol	2129.95		NIST Webbook
rinpol	2146.71		NIST Webbook
rinpol	2146.94		NIST Webbook
rinpol	2154.90		NIST Webbook
rinpol	2122.01		NIST Webbook
rinpol	2146.94		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R288612&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: 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

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