

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

Inchi: InChI=1S/C15H28ClN5/c1-7-9-14(3,4)20-12-17-11(16)18-13(19-12)21-15(5,6)10-8-2/h7-
InchiKey: ZBYDEMSHEGHUSN-UHFFFAOYSA-N
Formula: C15H28ClN5
SMILES: CCCC(C)(C)Nc1nc(Cl)nc(NC(C)(C)CCC)n1
Mol. weight [g/mol]: 313.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.88		Crippen Method
logp	4.506		Crippen Method
mcvol	260.590	ml/mol	McGowan Method
rinpol	2111.91		NIST Webbook
rinpol	2125.36		NIST Webbook
rinpol	2111.91		NIST Webbook
rinpol	2145.20		NIST Webbook
rinpol	2111.91		NIST Webbook
rinpol	2125.36		NIST Webbook
rinpol	2131.74		NIST Webbook
rinpol	2143.00		NIST Webbook
rinpol	2125.36		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R288598&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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