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

Inchi: InChI=1S/C13H24ClN5/c1-7-12(3,4)18-10-15-9(14)16-11(17-10)19-13(5,6)8-2/h7-8H2,1-

InchiKey: SPRRQTAXTOUPFY-UHFFFAOYSA-N

Formula: C13H24ClN5

SMILES: CCC(C)(C)Nc1nc(Cl)nc(NC(C)(C)CC)n1

Mol. weight [g/mol]: 285.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.04		Crippen Method
logp	3.726		Crippen Method
mcvol	232.410	ml/mol	McGowan Method
rinpol	1959.48		NIST Webbook
rinpol	2002.28		NIST Webbook
rinpol	1959.48		NIST Webbook
rinpol	2002.28		NIST Webbook
rinpol	2022.69		NIST Webbook
rinpol	1959.48		NIST Webbook
rinpol	2002.28		NIST Webbook
rinpol	1979.87		NIST Webbook
rinpol	1990.29		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R288607&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
rinpol: Non-polar retention indices