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

Inchi: InChI=1S/C17H32ClN5/c1-11(9-16(3,4)5)19-14-21-13(18)22-15(23-14)20-12(2)10-17(6,7
InchiKey: MFORFBJBHLBNSR-UHFFFAOYSA-N
Formula: C17H32ClN5
SMILES: CC(CC(C)(C)C)Nc1nc(Cl)nc(NC(C)CC(C)(C)C)n1
Mol. weight [g/mol]: 341.92

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.24		Crippen Method
logp	4.998		Crippen Method
mcvol	288.770	ml/mol	McGowan Method
rinpol	2235.62		NIST Webbook
rinpol	2251.95		NIST Webbook
rinpol	2235.62		NIST Webbook
rinpol	2255.14		NIST Webbook
rinpol	2271.67		NIST Webbook
rinpol	2251.95		NIST Webbook
rinpol	2271.48		NIST Webbook
rinpol	2235.62		NIST Webbook
rinpol	2251.95		NIST Webbook

Sources

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=R288632&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices