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

Inchi: InChI=1S/C17H32ClN5/c1-11(2)9-16(5,6)22-14-19-13(18)20-15(21-14)23-17(7,8)10-12(3

InchiKey: RYHPXBYKSKCPSV-UHFFFAOYSA-N

Formula: C17H32ClN5

SMILES: CC(C)CC(C)(C)Nc1nc(Cl)nc(NC(C)(C)CC(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	2205.28		NIST Webbook
rinpol	2258.03		NIST Webbook
rinpol	2205.28		NIST Webbook
rinpol	2224.74		NIST Webbook
rinpol	2234.95		NIST Webbook
rinpol	2258.03		NIST Webbook
rinpol	2277.47		NIST Webbook
rinpol	2205.28		NIST Webbook
rinpol	2258.03		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=R288583&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