6-Chloro-N,N'-(1-methylbutyl)-[1,3,5]triazine-2,4-di

Other names: 2,4-bis(1-methylbutyl-amino)-6-chloro-s-triazine
Inchi: InChI=1S/C13H24ClN5/c1-5-7-9(3)15-12-17-11(14)18-13(19-12)16-10(4)8-6-2/h9-10H,5-
InchiKey: OMKBSBCPFYUTLC-UHFFFAOYSA-N
Formula: C13H24ClN5
SMILES: CCCC(C)Nc1nc(Cl)nc(NC(C)CCC)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	2040.76		NIST Webbook
rinpol	2066.83		NIST Webbook
rinpol	2086.42		NIST Webbook
rinpol	2066.83		NIST Webbook
rinpol	2066.83		NIST Webbook
rinpol	2021.48		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R288652&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