1,3,5-Triazine-2,4-diamine, 6-chloro-N,N'-bis(1,1-dimethylethyl)-

Other names: 1,3,5-Triazine, 2,4-diamine, N,N'-bis(1,1-dimethylethyl)-)-6-chloro-
1,3,5-Triazine, 2,4-bis(tert-butylamino)-6-chloro-
s-Triazine, 2-chloro-4,6-bis-(tert.-butylamino)

Inchi: InChI=1S/C11H20ClN5/c1-10(2,3)16-8-13-7(12)14-9(15-8)17-11(4,5)6/h1-6H3,(H2,13,14

InchiKey: FOCLPSNTXOGURM-UHFFFAOYSA-N

Formula: C11H20ClN5

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

Mol. weight [g/mol]: 257.76

CAS: 39605-42-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.21		Crippen Method
logp	2.946		Crippen Method
mcvol	204.230	ml/mol	McGowan Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C39605420&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume