N-tert-Butyl-N'-acetyl-6-chloro-1,3,5-triazine-2,4-di

Other names: 1,3,5-Triazine-2,4-diamine, 6-chloro-N-(1,1-dimethylethyl)-N'-acetyl-
6-Chloro-N-(2-methyl-2-propanyl)-N'-acetyl-1,3,5-triazine-2,4-diamine
N-(4-Acetamino-6-chloro-1,3,5-triazin-2-yl)-N-(tert-butyl)amine
2-Acetamino-4-tert-butylamino-6-chloro-1,3,5-triazine
Inchi: InChI=1S/C9H14ClN5O/c1-5(16)11-7-12-6(10)13-8(14-7)15-9(2,3)4/h1-4H3,(H2,11,12,13
InchiKey: DYRSLXURNMQEOR-UHFFFAOYSA-N
Formula: C9H14ClN5O
SMILES: CC(=O)Nc1nc(Cl)nc(NC(C)(C)C)n1
Mol. weight [g/mol]: 243.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.03		Crippen Method
logp	1.694		Crippen Method
mcvol	177.620	ml/mol	McGowan Method
rinpol	1898.00		NIST Webbook
rinpol	1898.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373108&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices