

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

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)1
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/ci9903071
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

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