

6-Chloro-N-sec-butyl-N'-acetyl-1,3,5-triazine-2,4-d

Other names:	N-sec-Butyl-N'-acetyl-6-chloro-1,3,5-triazine-2,4-diamine
Inchi:	InChI=1S/C9H14ClN5O/c1-4-5(2)11-8-13-7(10)14-9(15-8)12-6(3)16/h5H,4H2,1-3H3,(H2
InchiKey:	ZORWFEGQUKCHHO-UHFFFAOYSA-N
Formula:	C9H14ClN5O
SMILES:	CCC(C)Nc1nc(Cl)nc(NC(C)=O)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
rinsol	1964.00		NIST Webbook
rinpol	1964.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U372980&Units=SI

Legend

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

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