

N2-Cyclopropyl-1,3,5-triazine-2,4,6-triamine N4,N6-diacetyl

Other names:	2,4-Diacetylamino-6-(cyclopropylamino)-s-triazine 2-Cyclopropylamino-4,6-diacetylamino-s-triazine
Inchi:	InChI=1S/C10H14N6O2/c1-5(17)11-8-14-9(12-6(2)18)16-10(15-8)13-7-3-4-7/h7H,3-4H2,
InchiKey:	LDRFWPALZPPMTA-UHFFFAOYSA-N
Formula:	C10H14N6O2
SMILES:	CC(=O)Nc1nc(NC(C)=O)nc(NC2CC2)n1
Mol. weight [g/mol]:	250.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.03		Crippen Method
logp	0.363		Crippen Method
mcvol	180.160	ml/mol	McGowan Method
rmpol	2337.00		NIST Webbook
rmpol	2337.00		NIST Webbook

Sources

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=U373432&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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