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

Other names: 2-Amino-4-cetylamino-6-(cyclopropylamino)-s-triazine
2-Cyclopropylamino-4-amino-6-acetylamino-s-triazine
Inchi: InChI=1S/C8H12N6O/c1-4(15)10-7-12-6(9)13-8(14-7)11-5-2-3-5/h5H,2-3H2,1H3,(H4,9,1
InchiKey: NLWFVDCAORFUAE-UHFFFAOYSA-N
Formula: C8H12N6O
SMILES: CC(=O)Nc1nc(N)nc(NC2CC2)n1
Mol. weight [g/mol]: 208.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.46		Crippen Method
logp	-0.014		Crippen Method
mcvol	150.410	ml/mol	McGowan Method
rinpol	2152.00		NIST Webbook
rinpol	2152.00		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=U373431&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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