

[(3S,4r,5s)-4-acetyloxy-5-(acetyloxymethyl)-2-(2,6-

acetate

InChI: InChI=1S/C16H20N6O7/c1-6(23)26-4-9-11(27-7(2)24)12(28-8(3)25)15(29-9)22-5-19-10-

InChIKey: SYQRSDUMMOZBJO-ORAFQZHNSA-N

Formula: C16H20N6O7

SMILES: CC(=O)OCC1OC(n2cnc3c(N)nc(N)nc32)C(OC(C)=O)C1OC(C)=O

Mol. weight [g/mol]: 408.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.23		Crippen Method
logp	-0.685		Crippen Method
mcvol	274.590	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6010448&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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