

9H-purine, 2,6-dichloro-9-beta-d-ribofuranosyl-, 2,3,5'-triacetate

InChI: InChI=1S/C16H16Cl2N4O7/c1-6(23)26-4-9-11(27-7(2)24)12(28-8(3)25)15(29-9)22-5-19-10-13-14-16
InChIKey: PYXZXWLFAMZVPY-UHFFFAOYSA-N

Formula: C16H16Cl2N4O7
SMILES: CC(=O)OCC1OC(n2cnc3c(Cl)nc(Cl)nc32)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 447.23
CAS: 3056-18-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	1.457		Crippen Method
mvol	279.110	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=C3056186&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
mvol: McGowan's characteristic volume

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