9H-purine, 2,6-difluoro-9-beta-d-xylofuranosyl-, 2',3',5'-triacetate

Inchi: InChI=1S/C16H16F2N4O7/c1-6(23)26-4-9-11(27-7(2)24)12(28-8(3)25)15(29-9)22-5-19-1
InchiKey: FOGUBSQHDZGAOK-ORAFQZHNSA-N
Formula: C16H16F2N4O7
SMILES: CC(=O)OCC1OC(n2cnc3c(F)nc(F)nc32)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 414.32
CAS: 18354-15-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.63		Crippen Method
logp	0.428		Crippen Method
mcvol	258.170	ml/mol	McGowan Method

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=C18354159&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