Allopurinol riboside, tris(trifluoroacetate)

Inchi: InChI=1S/C16H9F9N4O8/c17-14(18,19)11(31)34-2-5-6(36-12(32)15(20,21)22)7(37-13(3
InchiKey: CNVLLYZVMIWSKX-UHFFFAOYSA-N
Formula: C16H9F9N4O8
SMILES: O=C(OCC1OC(n2ncc3c(=O)[nH]cnc32)C(OC(=O)C(F)(F)F)C1OC(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 556.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.83		Crippen Method
logp	0.589		Crippen Method
mcvol	276.430	ml/mol	McGowan Method
rinpol	2303.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U375681&Units=SI

Legend

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