N-Methyl-1-deoxynojirimycin, tetrakis(trifluoroacetate)

Inchi: InChI=1S/C15H11F12NO8/c1-28-2-5(34-9(30)13(19,20)21)7(36-11(32)15(25,26)27)6(35
InchiKey: WVNHHIIANZADCI-UHFFFAOYSA-N
Formula: C15H11F12NO8
SMILES: CN1CC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1COC(=O)C(F)(F)F
Mol. weight [g/mol]: 561.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	1.828		Crippen Method
mcvol	272.330	ml/mol	McGowan Method
rinpol	1308.50		NIST Webbook
rinpol	1308.50		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=U380217&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.