Acetylgynuramine

Inchi: InChI=1S/C20H27NO7/c1-4-13-9-15(11-26-12(2)22)20(3,25)19(24)27-10-14-5-7-21-8-6-1
InchiKey: JAWLPMQZKYJXPI-JNALBJKISA-N
Formula: C20H27NO7
SMILES: CC=C1CC(COC(C)=O)C(C)(O)C(=O)OCC2=CCN3CCC(OC1=O)C23
Mol. weight [g/mol]: 393.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.10		Crippen Method
logp	0.736		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
rinpol	2610.00		NIST Webbook
rinpol	2678.00		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=R178095&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

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