

7-acetylcopsamine

Inchi: InChI=1S/C17H27NO6/c1-10(2)17(22,11(3)19)16(21)23-9-13-5-7-18-8-6-14(15(13)18)24
InchiKey: RKDOFSJTBIDAHX-OJBCNAABSA-N
Formula: C17H27NO6
SMILES: CC(=O)OC1CCN2CC=C(COC(=O)C(O)(C(C)C)C(C)O)C12
Mol. weight [g/mol]: 341.40

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.61 | | Crippen Method |
| logp | 0.244 | | Crippen Method |
| mcvol | 260.970 | ml/mol | McGowan Method |
| rinpol | 2230.00 | | NIST Webbook |
| rinpol | 2230.00 | | NIST Webbook |
| rinpol | 2239.00 | | NIST Webbook |
| rinpol | 2239.00 | | NIST Webbook |

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=R227815&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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<https://www.cheméo.com/cid/26-004-8/7-acetylcopsamine.pdf>

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