

3«beta»,13«alpha»-Dihydroxylupanine

Inchi: InChI=1S/C15H24N2O3/c18-11-1-2-12-9-5-10(6-16(12)8-11)15-13(19)3-4-14(20)17(15)7
InchiKey: OGGQJECTJUMTNM-BIUPMWDMSA-N
Formula: C15H24N2O3
SMILES: O=C1CCC(O)C2C3CC(CN12)C1CCC(O)CN1C3
Mol. weight [g/mol]: 280.36

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.09 | | Crippen Method |
| logp | -0.187 | | Crippen Method |
| mcvol | 212.040 | ml/mol | McGowan Method |
| rinsol | 2530.00 | | NIST Webbook |
| rinsol | 2508.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R264012&Units=SI>

Legend

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

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