

4,13-Dihydroxylupanine

Inchi: InChI=1S/C15H26N2O2/c18-14-6-3-5-13-11-8-10(9-17(13)14)12-4-1-2-7-16(12)15(11)19
InchiKey: NXRUZNUZJRPNHB-ZTQFERANSA-N
Formula: C15H26N2O2
SMILES: OC1CCCC2C3CC(CN12)C1CCCCN1C3O
Mol. weight [g/mol]: 266.38

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.30 | | Crippen Method |
| logp | 0.982 | | Crippen Method |
| mcvol | 210.470 | ml/mol | McGowan Method |
| rinpola | 2510.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R109143&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/67-968-4/4-13-Dihydroxylupanine.pdf>

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