

9-Hydroxyheptanoylretronecine

Inchi: InChI=1S/C15H25NO3/c1-2-3-4-5-6-14(18)19-11-12-7-9-16-10-8-13(17)15(12)16/h7,13,14,15,16,17,18,19
InchiKey: HUVCHNUWYBYZJU-CFMCSPISA-N
Formula: C15H25NO3
SMILES: CCCCCC(=O)OCC1=CCN2CCC(O)C12
Mol. weight [g/mol]: 267.36

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.66 | | Crippen Method |
| logp | 1.875 | | Crippen Method |
| mcvol | 219.480 | ml/mol | McGowan Method |
| rinpol | 2039.00 | | NIST Webbook |
| rinpol | 2039.00 | | 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=R405268&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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