

Intermedine

Inchi: InChI=1S/C15H25NO5/c1-9(2)15(20,10(3)17)14(19)21-8-11-4-6-16-7-5-12(18)13(11)16/
InchiKey: SFVVQRJOGUKCEG-GVUJHPQVSA-N
Formula: C15H25NO5
SMILES: CC(C)C(O)(C(=O)OCC1=CCN2CCC(O)C12)C(C)O
Mol. weight [g/mol]: 299.36

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.17 | | Crippen Method |
| logp | -0.327 | | Crippen Method |
| mcvol | 231.220 | ml/mol | McGowan Method |
| rinpol | 2133.00 | | NIST Webbook |
| rinpol | 2130.00 | | NIST Webbook |
| rinpol | 2131.00 | | NIST Webbook |
| rinpol | 2130.00 | | NIST Webbook |
| rinpol | 2133.00 | | 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=R178233&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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