

Ipanguline D5

Inchi: InChI=1S/C15H25NO6/c1-9(22-10(2)17)15(3,20)14(19)21-8-11-4-6-16-7-5-12(18)13(11)
InchiKey: NWXBPCGWPSVFTO-CVARFHGKSA-N
Formula: C15H25NO6
SMILES: CC(=O)OC(C)C(C)(O)C(=O)OCC1CCN2CCC(O)C12
Mol. weight [g/mol]: 315.36

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -0.92 | | Crippen Method |
| logp | -0.313 | | Crippen Method |
| mcvol | 237.090 | ml/mol | McGowan Method |
| rinpol | 2157.00 | | NIST Webbook |
| rinpol | 2157.00 | | NIST Webbook |
| rinpol | 2157.00 | | 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=R395032&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

Latest version available from:

<https://www.chemeo.com/cid/48-608-4/lpanguline-D5.pdf>

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