

3«beta»-(Hydroxy-2-Methylbutyroxyl)tropane

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|-----------------------------|--|
| Inchi: | InChI=1S/C13H23NO3/c1-4-13(2,16)12(15)17-11-7-9-5-6-10(8-11)14(9)3/h9-11,16H,4-8 |
| InchiKey: | BDPJWSRHFVSVHZ-DQFQTKLBSA-N |
| Formula: | C13H23NO3 |
| SMILES: | CCC(C)(O)C(=O)OC1CC2CCC(C1)N2C |
| Mol. weight [g/mol]: | 241.33 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.20 | | Crippen Method |
| logp | 1.316 | | Crippen Method |
| mcvol | 195.600 | ml/mol | McGowan Method |
| rinsol | 1705.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R509652&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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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