

13-Methylbutyryloxy-lupanine

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|-----------------------------|--|
| Inchi: | InChI=1S/C20H32N2O3/c1-13(2)8-20(24)25-17-5-7-21-15(11-17)9-14-10-16(21)12-18-19 |
| InchiKey: | APCPIFZNNFGYDW-UHFFFAOYSA-N |
| Formula: | C20H32N2O3 |
| SMILES: | CC(C)CC(=O)OC1CCN2C(C1)CC1CC2CC2C(=O)CCCN12 |
| Mol. weight [g/mol]: | 348.48 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.37 | | Crippen Method |
| logp | 2.377 | | Crippen Method |
| mcvol | 278.190 | ml/mol | McGowan Method |
| rinpola | 2655.00 | | 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=R261251&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 |
| rinpola: | Non-polar retention indices |

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<https://www.chemeo.com/cid/22-509-2/13-Methylbutyryloxy-lupanine.pdf>

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