# 13-Methylbutyryloxy-lupanine

**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 |
| rinpol | 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

**rinpol:** Non-polar retention indices