

4.alpha.-Angeloyloxy-3.beta.-hydroxylupanine

InChI: InChI=1S/C20H28N2O5/c1-3-11(2)20(26)27-15-9-16(23)22-10-12-8-13(17(22)18(15)24)19(25)21-7-5-4-6-14(12)21/h3,12-15,17-18,24H,4-10H2,1-2H3/b11-3-/t12?,13?,14?,15-,17?,18+/m0/s1

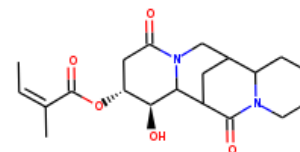
InChI Key: BRCTWJKFAXRQBQ-KPQUXXMESA-N

Formula: C20H28N2O5

SMILES:

CC=C(C)C(=O)OC1CC(=O)N2CC3CC(C(=O)N4CCCCC34)C2C1O

Molecular Weight: 376.45



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	0.857		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H28N2O5/c1-3-11\(2\)20\(26\)27-15-9-16\(23\)22-10-12-8-13\(17\(22\)18\(15\)24\)19\(25\)21-7-5-4-6-14\(12\)21/h3,12-15,17-18,24H,4-10H2,1-2H3/b11-3-/t12?,13?,14?,15-,17?,18+/m0/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H28N2O5/c1-3-11(2)20(26)27-15-9-16(23)22-10-12-8-13(17(22)18(15)24)19(25)21-7-5-4-6-14(12)21/h3,12-15,17-18,24H,4-10H2,1-2H3/b11-3-/t12?,13?,14?,15-,17?,18+/m0/s1)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

Latest version available from:

<https://old.cheméo.com/cid/64-476-3/4.alpha.-Angeloyloxy-3.beta.-hydroxylupanine>

Generated by Cheméo on Sun, 26 Jun 2022 20:49:56 +0000.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.