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

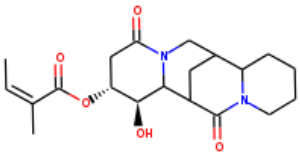
InChI: InChI=1S/C20H28N2O5/c1-3-11(2)20(26)27-15-9-16(23)22-10-12-8-13(17(22)18(15)24)19(25)21-7-5-4-6-14(12)21/h3,12-15,17-18,24H,4-10H2,1-2H3/b11-3-/t12?,13?,14?,15-,17?,18+/m0/s1

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$_{oct/wat}$	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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

***log*P$_{oct/wat}$**: Octanol/Water partition coefficient .