

13a-Acetoxyilupanine

Other names: 13-Acetyloxyilupanine
Inchi: InChI=1S/C17H26N2O3/c1-11(20)22-14-5-6-18-9-12-7-13(16(18)8-14)10-19-15(12)3-2-4
InchiKey: ZFTSMQKTSQDNDJ-UHFFFAOYSA-N
Formula: C17H26N2O3
SMILES: CC(=O)OC1CCN2CC3CC(CN4C(=O)CCCC34)C2C1
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.15		Crippen Method
logp	1.413		Crippen Method
mcvol	235.920	ml/mol	McGowan Method
rinpol	2450.00		NIST Webbook
rinpol	2450.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U383541&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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