3«beta»-Propanyloxylupanine

Inchi: InChI=1S/C18H28N2O3/c1-2-17(22)23-15-6-7-16(21)20-11-12-9-13(18(15)20)10-19-8-4-
InchiKey: ORQVQUZMVCLDKD-GNFNDJEDSA-N
Formula: C18H28N2O3
SMILES: CCC(=O)OC1CCC(=O)N2CC3CC(CN4CCCCC34)C12
Mol. weight [g/mol]: 320.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	1.803		Crippen Method
mcvol	250.010	ml/mol	McGowan Method
rinpol	2590.00		NIST Webbook
rinpol	2590.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R264047&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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