Opipramol, acetylated

Inchi: InChI=1S/C25H33N3O2/c1-21(29)30-20-19-27-17-15-26(16-18-27)13-6-14-28-24-9-4-2-7

InchiKey: JXJVSQWMXWLOKF-UHFFFAOYSA-N

Formula: C25H33N3O2

SMILES: CC(=O)OCCN1CCN(CCCN2c3ccccc3CCc3ccccc32)CC1

Mol. weight [g/mol]: 407.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.92		Crippen Method
logp	3.494		Crippen Method
mcvol	331.250	ml/mol	McGowan Method
rinpol	3171.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R311178&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