Cinnarizine M (carbinol), acetylated

Inchi: InChI=1S/C28H30N2O2/c1-24(31)32-28(26-15-7-3-8-16-26,27-17-9-4-10-18-27)30-22-20

InchiKey: JBYBHZSAOUIVHG-KAMYIIQDSA-N

Formula: C28H30N2O2

SMILES: CC(=O)OC(c1ccccc1)(c1ccccc1)N1CCN(CC=Cc2ccccc2)CC1

Mol. weight [g/mol]: 426.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.54		Crippen Method
logp	4.782		Crippen Method
mcvol	346.340	ml/mol	McGowan Method
rinpol	1700.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R536179&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices