Cinnarizine M (N-desalkyl-hydroxy), acetylated

Inchi: InChI=1S/C21H24N2O3/c1-16(24)22-12-14-23(15-13-22)21(18-6-4-3-5-7-18)19-8-10-20(
InchiKey: KJTZNYZQURJGTA-UHFFFAOYSA-N
Formula: C21H24N2O3
SMILES: CC(=O)Oc1ccc(C(c2ccccc2)N2CCN(C(C)=O)CC2)cc1
Mol. weight [g/mol]: 352.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Crippen Method
logp	2.865		Crippen Method
mcvol	277.340	ml/mol	McGowan Method
rinpol	2580.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R536233&Units=SI

Legend

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