Cyproheptadine M (nor, OH), acetylated

Inchi: InChI=1S/C24H23NO3/c1-16(26)25-13-11-19(12-14-25)24-22-6-4-3-5-18(22)7-8-20-15-2
InchiKey: ZZNCEZMUVQRSLX-UHFFFAOYSA-N
Formula: C24H23NO3
SMILES: CC(=O)Oc1ccc2c(c1)C=Cc1ccccc1C2=C1CCN(C(C)=O)CC1
Mol. weight [g/mol]: 373.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.93		Crippen Method
logp	4.540		Crippen Method
mcvol	290.170	ml/mol	McGowan Method
rinpol	3060.00		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=R120615&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