Cyproheptadine M (nor), acetylated

Inchi: InChI=1S/C22H21NO/c1-16(24)23-14-12-19(13-15-23)22-20-8-4-2-6-17(20)10-11-18-7-3
InchiKey: UDWGIXOMTFQKAU-UHFFFAOYSA-N
Formula: C22H21NO
SMILES: CC(=O)N1CCC(=C2c3ccccc3C=Cc3ccccc32)CC1
Mol. weight [g/mol]: 315.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.61		Crippen Method
logp	4.615		Crippen Method
mcvol	254.550	ml/mol	McGowan Method
rinpol	2920.00		NIST Webbook
rinpol	2920.00		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=R120600&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

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