

Terfenadine M (N-des-alkyl, -H₂O), acetylated

Inchi: InChI=1S/C20H21NO/c1-16(22)21-14-12-19(13-15-21)20(17-8-4-2-5-9-17)18-10-6-3-7-1
InchiKey: KVXMZFYFJCSLSB-UHFFFAOYSA-N
Formula: C₂₀H₂₁NO
SMILES: CC(=O)N1CCC(=C(c2ccccc2)c2ccccc2)CC1
Mol. weight [g/mol]: 291.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.76		Crippen Method
logp	4.131		Crippen Method
mcvol	241.530	ml/mol	McGowan Method
rinsol	2550.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R120744&Units=SI>

Legend

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

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