

# Terfenadine M (-2H<sub>2</sub>O)

**Inchi:** InChI=1S/C32H37N/c1-32(2,3)30-19-17-26(18-20-30)12-10-11-23-33-24-21-29(22-25-33)  
**InchiKey:** XTBJPNHHVAIUJX-BENRWUELSA-N  
**Formula:** C<sub>32</sub>H<sub>37</sub>N  
**SMILES:** CC(C)(C)c1ccc(C=CCCN2CCC(=C(c3ccccc3)c3ccccc3)CC2)cc1  
**Mol. weight [g/mol]:** 435.64

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.77		Crippen Method
logp	7.985		Crippen Method
mcvol	380.980	ml/mol	McGowan Method
rinpola	3460.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R314602&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

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

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