Brompheniramine M (bis-nor), acetylated

Inchi: InChI=1S/C16H17BrN2O/c1-12(20)18-11-9-15(16-4-2-3-10-19-16)13-5-7-14(17)8-6-13/h
InchiKey: KEKRTYBPZPYZSJ-UHFFFAOYSA-N
Formula: C16H17BrN2O
SMILES: CC(=O)NCCC(c1ccc(Br)cc1)c1ccccn1
Mol. weight [g/mol]: 333.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.10		Crippen Method
logp	3.502		Crippen Method
mcvol	227.810	ml/mol	McGowan Method
rinpol	2170.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R120511&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: 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
rinpol: Non-polar retention indices