Phenindamine M (OH), acetylated

Inchi: InChI=1S/C20H20N2O2/c1-14(23)24-16-8-9-19-18(12-16)17-10-11-21(2)13-20(17)22(19
InchiKey: CRNMOQJJUILRJK-UHFFFAOYSA-N
Formula: C20H20N2O2
SMILES: CC(=O)Oc1ccc2c(c1)c1c(n2-c2ccccc2)CN(C)CC1
Mol. weight [g/mol]: 320.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.81		Crippen Method
logp	3.544		Crippen Method
mcvol	246.520	ml/mol	McGowan Method
rinpol	2580.00		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=R120695&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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