Phenindamine M (nor, OH), acetylated

Inchi: InChI=1S/C21H20N2O3/c1-14(24)22-11-10-18-19-12-17(26-15(2)25)8-9-20(19)23(21(18
InchiKey: BKGSMXJXYZQESK-UHFFFAOYSA-N
Formula: C21H20N2O3
SMILES: CC(=O)Oc1ccc2c(c1)c1c(n2-c2ccccc2)CN(C(C)=O)CC1
Mol. weight [g/mol]: 348.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.00		Crippen Method
logp	3.460		Crippen Method
mcvol	262.180	ml/mol	McGowan Method
rinpol	3000.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R120680&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