

Phenindamine M (nor), acetylated

Inchi:	InChI=1S/C19H18N2O/c1-14(22)20-12-11-17-16-9-5-6-10-18(16)21(19(17)13-20)15-7-3
InchiKey:	NEPPNZJETYGNHF-UHFFFAOYSA-N
Formula:	C19H18N2O
SMILES:	CC(=O)N1CCc2c(n(-c3ccccc3)c3ccccc23)C1
Mol. weight [g/mol]:	290.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	3.535		Crippen Method
mcvol	226.560	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R120675&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

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<https://www.chemeo.com/cid/97-755-7/Phenindamine-M-nor-acetylated.pdf>

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