Phenindamine

Other names:	1H-Indeno[2,1-c]pyridine, 2,3,4,9-tetrahydro-2-methyl-9-phenyl- NU 1504 Thephorin 2,3,4,9-Tetrahydro-2-methyl-9-phenyl-1H-indeno[2,1-c]pyridine Fenindamina Phenindiamine
Inchi:	InChI=1S/C19H19N/c1-20-12-11-16-15-9-5-6-10-17(15)19(18(16)13-20)14-7-3-2-4-8-14/
InchiKey:	ISFHAYSTHMVOJR-UHFFFAOYSA-N
Formula:	C19H19N
SMILES:	CN1CCC2=C(C1)C(c1ccccc1)c1ccccc12
Mol. weight [g/mol]:	261.36
CAS:	82-88-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.39		Crippen Method
logp	3.921		Crippen Method
mcvol	215.010	ml/mol	McGowan Method
rinpol	2109.00		NIST Webbook
rinpol	2167.00		NIST Webbook
rinpol	2109.00		NIST Webbook
rinpol	2158.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2147.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82882&Units=SI
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

Legend

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