

diphenyl-nicotinamide

Inchi:	InChI=1S/C18H14N2O/c21-18(15-8-7-13-19-14-15)20(16-9-3-1-4-10-16)17-11-5-2-6-12-
InchiKey:	FYFWGHVSOVRQBY-UHFFFAOYSA-N
Formula:	C18H14N2O
SMILES:	O=C(c1cccnc1)N(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	274.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.91		Crippen Method
logp	4.060		Crippen Method
mcvol	214.730	ml/mol	McGowan Method
rinpole	2570.00		NIST Webbook

Sources

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=R211033&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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<https://www.chemeo.com/cid/97-394-8/diphenyl-nicotinamide.pdf>

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