N-(1,2-Diphenylethyl)nicotinamide

Inchi: InChI=1S/C20H18N2O/c23-20(18-12-7-13-21-15-18)22-19(17-10-5-2-6-11-17)14-16-8-3-
InchiKey: DWODOIKZDGJOPQ-UHFFFAOYSA-N
Formula: C20H18N2O
SMILES: O=C(NC(Cc1ccccc1)c1ccccc1)c1cccnc1
Mol. weight [g/mol]: 302.37
CAS: 553-06-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	3.795		Crippen Method
mcvol	242.910	ml/mol	McGowan Method
rinpol	2574.00		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=C553060&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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