1H-Pyrrole, 2,4-diphenyl-

Other names:	Pyrrole, 2,4-diphenyl- 2,4-Diphenylpyrrole 2,4-Diphenyl-1H-pyrrole
Inchi:	InChI=1S/C16H13N/c1-3-7-13(8-4-1)15-11-16(17-12-15)14-9-5-2-6-10-14/h1-12,17H
InchiKey:	FSBPQTRUHOMNPG-UHFFFAOYSA-N
Formula:	C16H13N
SMILES:	c1ccc(-c2c[nH]c(-c3ccccc3)c2)cc1
Mol. weight [g/mol]:	219.28
CAS:	3274-56-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.90		Crippen Method
logp	3.867		Crippen Method
mcvol	179.300	ml/mol	McGowan Method
rinpol	1790.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1790.00		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=C3274564&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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