1,4-Phenylenediamine, N,N'-bis((4-pyridyl)methylene)-

Inchi: InChI=1S/C18H14N4/c1-2-18(22-14-16-7-11-20-12-8-16)4-3-17(1)21-13-15-5-9-19-10-6-

InchiKey: PBUIXULEGNITAX-UHFFFAOYSA-N

Formula: C18H14N4

SMILES: C(=Nc1ccc(N=Cc2ccncc2)cc1)c1ccncc1

Mol. weight [g/mol]: 286.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.73		Crippen Method
logp	3.978		Crippen Method
mcvol	224.520	ml/mol	McGowan Method
rinpol	3061.00		NIST Webbook
rinpol	3061.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U376688&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

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.