4-(4-Phenoxybutyl)pyridine

Inchi: InChI=1S/C15H17NO/c1-2-7-15(8-3-1)17-13-5-4-6-14-9-11-16-12-10-14/h1-3,7-12H,4-6,
InchiKey: RJJZWSYLKARLJM-UHFFFAOYSA-N
Formula: C15H17NO
SMILES: c1ccc(OCCCCc2ccncc2)cc1
Mol. weight [g/mol]: 227.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.23		Crippen Method
logp	3.483		Crippen Method
mcvol	190.540	ml/mol	McGowan Method
rinpol	1985.00		NIST Webbook
rinpol	1985.00		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=R545509&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

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