2-n-Pentyl-4-methoxyquinoline

Inchi: InChI=1S/C16H21N/c1-3-5-6-9-14-12-13(4-2)15-10-7-8-11-16(15)17-14/h7-8,10-12H,3-6
InchiKey: UWUREZICVFHTMU-UHFFFAOYSA-N
Formula: C16H21N
SMILES: CCCCCc1cc(CC)c2ccccc2n1
Mol. weight [g/mol]: 227.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.90		Crippen Method
logp	4.530		Crippen Method
mcvol	203.060	ml/mol	McGowan Method
rinpol	1927.00		NIST Webbook
rinpol	1927.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R398284&Units=SI
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

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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