3,5-dibutyl-2-pentyl-pyridine

Other names: 2-pentyl-3,5-dibutylpyridine
Inchi: InChI=1S/C18H31N/c1-4-7-10-13-18-17(12-9-6-3)14-16(15-19-18)11-8-5-2/h14-15H,4-13
InchiKey: QZKIFXRIRJFASX-UHFFFAOYSA-N
Formula: C18H31N
SMILES: CCCCCc1ncc(CCCC)cc1CCCC
Mol. weight [g/mol]: 261.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.58		Crippen Method
logp	5.499		Crippen Method
mcvol	250.700	ml/mol	McGowan Method
rinpol	1919.00		NIST Webbook
rinpol	1918.00		NIST Webbook
rinpol	1919.00		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=R268069&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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