

2-butyl-3,5-dipropyl-pyridine

Inchi: InChI=1S/C15H25N/c1-4-7-10-15-14(9-6-3)11-13(8-5-2)12-16-15/h11-12H,4-10H2,1-3H3
InchiKey: GJOWJMJVNFVZLN-UHFFFAOYSA-N
Formula: C15H25N
SMILES: CCCCc1ncc(CCC)cc1CCC
Mol. weight [g/mol]: 219.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.32		Crippen Method
logp	4.329		Crippen Method
mcvol	208.430	ml/mol	McGowan Method
rinpole	1643.00		NIST Webbook
rinpole	1643.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R268049&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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