

3,5-dipentyl-2-hexyl-pyridine

Inchi: InChI=1S/C21H37N/c1-4-7-10-13-16-21-20(15-12-9-6-3)17-19(18-22-21)14-11-8-5-2/h17
InchiKey: HHSSUILMGDVUQU-UHFFFAOYSA-N
Formula: C₂₁H₃₇N
SMILES: CCCCCCc1ncc(CCCCC)cc1CCCCC
Mol. weight [g/mol]: 303.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.83		Crippen Method
logp	6.670		Crippen Method
mcvol	292.970	ml/mol	McGowan Method
rinpol	2200.00		NIST Webbook
rinpol	2200.00		NIST Webbook

Sources

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=R268074&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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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<https://www.chemeo.com/cid/72-595-2/3-5-dipentyl-2-hexyl-pyridine.pdf>

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