1,4-Dipentylisoquinoline

Inchi: InChI=1S/C19H27N/c1-3-5-7-11-16-15-20-19(14-8-6-4-2)18-13-10-9-12-17(16)18/h9-10,
InchiKey: UKODNDSPGMOPGN-UHFFFAOYSA-N
Formula: C19H27N
SMILES: CCCCCc1cnc(CCCCC)c2ccccc12
Mol. weight [g/mol]: 269.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.16		Crippen Method
logp	5.700		Crippen Method
mcvol	245.330	ml/mol	McGowan Method
rinpol	2150.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R545376&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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