

1,4-Dibutylisoquinoline

Inchi: InChI=1S/C17H23N/c1-3-5-9-14-13-18-17(12-6-4-2)16-11-8-7-10-15(14)16/h7-8,10-11,13-15,17-18
InchiKey: BBCA00GKWQFZTI-UHFFFAOYSA-N
Formula: C17H23N
SMILES: CCCCc1cnc(CCCC)c2ccccc12
Mol. weight [g/mol]: 241.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.32		Crippen Method
logp	4.920		Crippen Method
mcvol	217.150	ml/mol	McGowan Method
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R545361&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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