

Quinoline, 2-butyl-3-propyl

Inchi:	InChI=1S/C16H21N/c1-3-5-10-15-13(8-4-2)12-14-9-6-7-11-16(14)17-15/h6-7,9,11-12H,3
InchiKey:	CZMKULCCAGNPDG-UHFFFAOYSA-N
Formula:	C16H21N
SMILES:	CCCCc1nc2cccc2cc1CCC
Mol. weight [g/mol]:	227.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.90		Crippen Method
logp	4.530		Crippen Method
mcvol	203.060	ml/mol	McGowan Method
ripol	2329.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R217422&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices

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<https://www.chemeo.com/cid/74-111-6/Quinoline-2-butyl-3-propyl.pdf>

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