Quinoline, 2-butyl-3-methyl-

Inchi: InChI=1S/C14H17N/c1-3-4-8-13-11(2)10-12-7-5-6-9-14(12)15-13/h5-7,9-10H,3-4,8H2,1-2
InchiKey: VVRRMVOHADLIPW-UHFFFAOYSA-N
Formula: C14H17N
SMILES: CCCCc1nc2ccccc2cc1C
Mol. weight [g/mol]: 199.29
CAS: 1531-62-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.16		Crippen Method
logp	3.886		Crippen Method
mcvol	174.880	ml/mol	McGowan Method
rinpol	1803.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1531620&Units=SI

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.