Quinoline, 3-butyl-2-methyl

Inchi: InChI=1S/C14H17N/c1-3-4-7-12-10-13-8-5-6-9-14(13)15-11(12)2/h5-6,8-10H,3-4,7H2,1-2
InchiKey: DWDMKPMAMRQPAI-UHFFFAOYSA-N
Formula: C14H17N
SMILES: CCCCc1cc2ccccc2nc1C
Mol. weight [g/mol]: 199.29

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	1695.00		NIST Webbook
rinpol	1708.00		NIST Webbook
rinpol	1695.00		NIST Webbook
ripol	2282.00		NIST Webbook
ripol	2309.00		NIST Webbook
ripol	2282.00		NIST Webbook
ripol	2309.00		NIST Webbook
ripol	2282.00		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=R37272&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
ripol:	Polar retention indices