Quinoline, 8-methyl-5-(1-methylethyl)

Inchi: InChI=1S/C13H15N/c1-9(2)11-7-6-10(3)13-12(11)5-4-8-14-13/h4-9H,1-3H3
InchiKey: CODKEMBFGZTJIG-UHFFFAOYSA-N
Formula: C13H15N
SMILES: Cc1ccc(C(C)C)c2cccnc12
Mol. weight [g/mol]: 185.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.70		Crippen Method
logp	3.667		Crippen Method
mcvol	160.790	ml/mol	McGowan Method
rinpol	1560.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1560.00		NIST Webbook
ripol	2135.00		NIST Webbook
ripol	2164.00		NIST Webbook
ripol	2135.00		NIST Webbook
ripol	2164.00		NIST Webbook
ripol	2135.00		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=R37286&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