Quinoline, 2-(2-methylpropyl)-

Other names:	Quinoline, 2-isobutyl- 2-Isobutylquinoline «alpha»-Isobutylquinoline
Inchi:	InChI=1S/C13H15N/c1-10(2)9-12-8-7-11-5-3-4-6-13(11)14-12/h3-8,10H,9H2,1-2H3
InchiKey:	FAQVGPWFQGGIPP-UHFFFAOYSA-N
Formula:	C13H15N
SMILES:	CC(C)Cc1ccc2ccccc2n1
Mol. weight [g/mol]:	185.26
CAS:	93-19-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.44		Crippen Method
logp	3.433		Crippen Method
mcvol	160.790	ml/mol	McGowan Method
rinpol	1515.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1501.00		NIST Webbook
ripol	2077.00		NIST Webbook
ripol	2048.00		NIST Webbook
ripol	2077.00		NIST Webbook
ripol	2048.00		NIST Webbook
ripol	2077.00		NIST Webbook
ripol	2048.00		NIST Webbook
ripol	2077.00		NIST Webbook
ripol	2048.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93196&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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