Quinoline, 2-pentyl

Other names: 2-Pentylquinoline
Inchi: InChI=1S/C14H17N/c1-2-3-4-8-13-11-10-12-7-5-6-9-14(12)15-13/h5-7,9-11H,2-4,8H2,1H
InchiKey: GMTGCIAJHZEUNB-UHFFFAOYSA-N
Formula: C14H17N
SMILES: CCCCCc1ccc2ccccc2n1
Mol. weight [g/mol]: 199.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.10		Crippen Method
logp	3.968		Crippen Method
mcvol	174.880	ml/mol	McGowan Method
rinpol	1650.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1664.00		NIST Webbook
ripol	2225.00		NIST Webbook
ripol	2249.00		NIST Webbook
ripol	2225.00		NIST Webbook
ripol	2249.00		NIST Webbook
ripol	2225.00		NIST Webbook
ripol	2249.00		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=R37268&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