Benzo[f]quinoline, 3-methyl-

Other names: «beta»-Naphthoquinaldine
3-Methylbenzo[f]quinoline
Inchi: InChI=1S/C14H11N/c1-10-6-8-13-12-5-3-2-4-11(12)7-9-14(13)15-10/h2-9H,1H3
InchiKey: SUHRSZJZYUCLOD-UHFFFAOYSA-N
Formula: C14H11N
SMILES: Cc1ccc2c(ccc3ccccc32)n1
Mol. weight [g/mol]: 193.24
CAS: 85-06-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.32		Crippen Method
logp	3.696		Crippen Method
mcvol	155.420	ml/mol	McGowan Method
rinpol	320.26		NIST Webbook
rinpol	320.77		NIST Webbook
rinpol	320.26		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C85063&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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