«alpha»-Naphthoquinoline

Inchi: InChI=1S/C17H11N/c1-2-6-13-11-17-15(9-12(13)5-1)10-14-7-3-4-8-16(14)18-17/h1-11H
InchiKey: JZYMCIPZZLIJKR-UHFFFAOYSA-N
Formula: C17H11N
SMILES: c1ccc2cc3nc4ccccc4cc3cc2c1
Mol. weight [g/mol]: 229.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.65		Crippen Method
logp	4.541		Crippen Method
mcvol	178.230	ml/mol	McGowan Method
rinpol	1720.00		NIST Webbook
rinpol	1720.00		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=R539970&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

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