Naphtho(2,3-h)quinoline

Other names: 1-Azabenz(a)anthracene
Inchi: InChI=1S/C17H11N/c1-2-5-14-11-16-15(10-13(14)4-1)8-7-12-6-3-9-18-17(12)16/h1-11H
InchiKey: JKJNHQJWGCHSHP-UHFFFAOYSA-N
Formula: C17H11N
SMILES: c1ccc2cc3c(ccc4cccnc43)cc2c1
Mol. weight [g/mol]: 229.28
CAS: 84-56-0

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	400.00		NIST Webbook
rinpol	400.00		NIST Webbook

Sources

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=C84560&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

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