

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:	<chem>c1ccc2cc3c(ccc4cccnc43)cc2c1</chem>
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/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/79-900-5/Naphtho-2-3-h-quinoline.pdf>

Generated by Cheméo on 2024-04-26 06:27:27.086314313 +0000 UTC m=+16402096.006891626.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.