

2-Azachrysene

Inchi:	InChI=1S/C17H11N/c1-2-4-14-12(3-1)5-7-17-15-9-10-18-11-13(15)6-8-16(14)17/h1-11H
InchiKey:	ACIUFBMENRNYHI-UHFFFAOYSA-N
Formula:	C17H11N
SMILES:	c1ccc2c(c1)ccc1c3ccncc3ccc21
Mol. weight [g/mol]:	229.28
CAS:	218-02-0

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	411.49		NIST Webbook
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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=C218020&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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<https://www.chemeo.com/cid/11-115-1/2-Azachrysene.pdf>

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