

10-Azabenz[a]pyrene

Inchi:	InChI=1S/C19H11N/c1-2-4-15-13(3-1)11-14-6-5-12-9-10-20-17-8-7-16(15)18(14)19(12)1
InchiKey:	PBJQMIJLHFAYGZ-UHFFFAOYSA-N
Formula:	C19H11N
SMILES:	c1ccc2c(c1)cc1ccc3ccnc4ccc2c1c34
Mol. weight [g/mol]:	253.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.87		Crippen Method
logp	5.132		Crippen Method
mcvol	191.250	ml/mol	McGowan Method
rinpol	455.40		NIST Webbook
rinpol	454.57		NIST Webbook
rinpol	455.40		NIST Webbook
rinpol	454.57		NIST Webbook
rinpol	455.40		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R21037&Units=SI
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

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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