

Benz[c]acridine, 7,9-dimethyl-

Other names:	7,9-Dimethylbenz[c]acridine
Inchi:	InChI=1S/C19H15N/c1-12-7-10-18-17(11-12)13(2)15-9-8-14-5-3-4-6-16(14)19(15)20-18/
InchiKey:	HEFJMRLDXHSXEP-UHFFFAOYSA-N
Formula:	C19H15N
SMILES:	<chem>Cc1ccc2nc3c(ccc4ccccc43)c(C)c2c1</chem>
Mol. weight [g/mol]:	257.33
CAS:	963-89-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.60		Crippen Method
logp	5.158		Crippen Method
mcvol	206.410	ml/mol	McGowan Method
rinpol	2769.00		NIST Webbook
rinpol	434.00		NIST Webbook
rinpol	438.32		NIST Webbook
rinpol	2769.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C963893&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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