

Benz[a]acridine, 1,10-dimethyl

Inchi: InChI=1S/C19H15N/c1-12-6-8-17-15(10-12)11-16-18(20-17)9-7-14-5-3-4-13(2)19(14)16/
InchiKey: AMVOWSHVCHBLEN-UHFFFAOYSA-N
Formula: C19H15N
SMILES: Cc1ccc2nc3ccc4cccc(C)c4c3cc2c1
Mol. weight [g/mol]: 257.33

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	2611.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R14587&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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