Benz[a]acridine, 5,7-dimethyl

Inchi: InChI=1S/C19H17N/c1-13-11-19-17(16-9-5-4-8-15(13)16)12-14-7-3-6-10-18(14)20(19)2/
InchiKey: CILOWUGLZFEBJS-UHFFFAOYSA-N
Formula: C19H17N
SMILES: CC1=C2C=CC=CC2C2=Cc3ccccc3N(C)C2=C1
Mol. weight [g/mol]: 259.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.32		Crippen Method
logp	4.476		Crippen Method
mcvol	210.710	ml/mol	McGowan Method
rinpol	2662.00		NIST Webbook
rinpol	438.38		NIST Webbook
rinpol	2662.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R14569&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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