

Benz[a]acridine, 2,10-dimethyl

Inchi: InChI=1S/C19H15N/c1-12-4-7-18-15(9-12)11-17-16-10-13(2)3-5-14(16)6-8-19(17)20-18/
InchiKey: WURDFEOGJYATFQ-UHFFFAOYSA-N
Formula: C19H15N
SMILES: Cc1ccc2nc3ccc4ccc(C)cc4c3cc2c1
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	2670.00		NIST Webbook
rinpol	2670.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R14591&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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

Latest version available from:

<https://www.cheméo.com/cid/40-734-2/Benz-a-acridine-2-10-dimethyl.pdf>

Generated by Cheméo on 2024-04-26 15:27:54.279269243 +0000 UTC m=+16434523.199846556.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.