Benz[a]acridine, 10-methyl-

Inchi: InChI=1S/C18H13N/c1-12-6-8-17-14(10-12)11-16-15-5-3-2-4-13(15)7-9-18(16)19-17/h2-
InchiKey: JNMYQFUNYDSRDY-UHFFFAOYSA-N
Formula: C18H13N
SMILES: Cc1ccc2nc3ccc4ccccc4c3cc2c1
Mol. weight [g/mol]: 243.30
CAS: 3781-67-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.13		Crippen Method
logp	4.850		Crippen Method
mcvol	192.320	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3781677&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