

Acridine, 9-phenyl-

Other names: 9-Phenylacridine
Inchi: InChI=1S/C19H13N/c1-2-8-14(9-3-1)19-15-10-4-6-12-17(15)20-18-13-7-5-11-16(18)19/h
InchiKey: MTRFEWTWIPAXLG-UHFFFAOYSA-N
Formula: C19H13N
SMILES: c1ccc(-c2c3ccccc3nc3ccccc23)cc1
Mol. weight [g/mol]: 255.31
CAS: 602-56-2

Physical Properties

Property code	Value	Unit	Source
ie	7.75	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
log10ws	-7.45		Crippen Method
logp	5.055		Crippen Method
mcvol	202.110	ml/mol	McGowan Method

Sources

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=C602562&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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