METHAPYRILENE

Inchi: InChI=1S/C14H19N3S/c1-16(2)8-9-17(11-13-6-10-18-12-13)14-5-3-4-7-15-14/h3-7,10,12
InchiKey: HNJJXZKZRAWDPF-UHFFFAOYSA-N
Formula: C14H19N3S
SMILES: CN(C)CCN(Cc1ccsc1)c1ccccn1
Mol. weight [g/mol]: 261.39

Physical Properties

Property code	Value	Unit	Source
ie	8.22	eV	Cheméo Relay (1.0)
log10ws	-2.64		Aqueous Solubility Prediction Method
logp	2.711		Crippen Method
mcvol	211.190	ml/mol	McGowan Method
tb	626.66	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C91792&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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