3-Methylquinoline-1-oxide

Inchi: InChI=1S/C10H9NO/c1-8-6-9-4-2-3-5-10(9)11(12)7-8/h2-7H,1H3
InchiKey: CBGUMTBCWWMBRV-UHFFFAOYSA-N
Formula: C10H9NO
SMILES: Cc1cc2ccccc2[n+]([O-])c1
Mol. weight [g/mol]: 159.18
CAS: 1873-55-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.28		Crippen Method
logp	1.782		Crippen Method
mcvol	124.390	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1873558&Units=SI

Legend

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