5-Phenyl-8-methoxy-quinoline

Inchi: InChI=1S/C16H13NO/c1-18-15-10-9-13(12-6-3-2-4-7-12)14-8-5-11-17-16(14)15/h2-11H,
InchiKey: DPPARAXTTAUTPS-UHFFFAOYSA-N
Formula: C16H13NO
SMILES: COc1ccc(-c2ccccc2)c2cccnc12
Mol. weight [g/mol]: 235.28
CAS: 116633-03-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.76		Crippen Method
logp	3.910		Crippen Method
mcvol	185.170	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=C116633035&Units=SI

Legend

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