2-Phenyl-3-methyl-4-hydroxy-quinoline

Inchi: InChI=1S/C16H13NO/c1-11-15(12-7-3-2-4-8-12)17-14-10-6-5-9-13(14)16(11)18/h2-10H,
InchiKey: WODRVCHVTSPANG-UHFFFAOYSA-N
Formula: C16H13NO
SMILES: Cc1c(-c2ccccc2)[nH]c2ccccc2c1=O
Mol. weight [g/mol]: 235.28
CAS: 6943-08-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.00		Crippen Method
logp	3.022		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=C6943084&Units=SI

Legend

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