

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/ci9903071
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

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