7-(4-ethyl-1-methyloctyl)-8-hydroxy-quinoline

Inchi: InChI=1S/C20H29NO/c1-4-6-8-16(5-2)11-10-15(3)18-13-12-17-9-7-14-21-19(17)20(18)2
InchiKey: YWACCMLWVBYNHR-UHFFFAOYSA-N
Formula: C20H29NO
SMILES: CCCCC(CC)CCC(C)c1ccc2cccnc2c1O
Mol. weight [g/mol]: 299.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.88		Crippen Method
logp	6.040		Crippen Method
mcvol	265.290	ml/mol	McGowan Method
rinpol	2295.00		NIST Webbook
rinpol	2296.00		NIST Webbook
rinpol	2295.00		NIST Webbook

Sources

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=R261088&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices