7-(2-ethylhexyl)-8-hydroxyquinoline

Inchi: InChI=1S/C17H23NO/c1-3-5-7-13(4-2)12-15-10-9-14-8-6-11-18-16(14)17(15)19/h6,8-11,
InchiKey: FOMHJBDTLRDQBH-UHFFFAOYSA-N
Formula: C17H23NO
SMILES: CCCCC(CC)Cc1ccc2cccnc2c1O
Mol. weight [g/mol]: 257.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.66		Crippen Method
logp	4.699		Crippen Method
mcvol	223.020	ml/mol	McGowan Method
rinpol	2076.00		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=R261073&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