2-(3',4'-Methylenedioxyphenylethyl)quinoline

Inchi: InChI=1S/C18H15NO2/c1-2-4-16-14(3-1)7-9-15(19-16)8-5-13-6-10-17-18(11-13)21-12-2
InchiKey: ZDRLPWFUZOCXJT-UHFFFAOYSA-N
Formula: C18H15NO2
SMILES: c1ccc2nc(CCc3ccc4c(c3)OCO4)ccc2c1
Mol. weight [g/mol]: 277.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.67		Crippen Method
logp	3.749		Crippen Method
mcvol	208.360	ml/mol	McGowan Method
rinpol	2515.00		NIST Webbook
rinpol	2515.00		NIST Webbook

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=R398259&Units=SI

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.