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

Inchi: InChI=1S/C19H19NO2/c1-21-18-12-8-14(13-19(18)22-2)7-10-16-11-9-15-5-3-4-6-17(15)
InchiKey: OXJATSFPAYFXMW-UHFFFAOYSA-N
Formula: C19H19NO2
SMILES: COc1ccc(CCc2ccc3ccccc3n2)cc1OC
Mol. weight [g/mol]: 293.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.70		Crippen Method
logp	4.037		Crippen Method
mcvol	233.310	ml/mol	McGowan Method
rinpol	2568.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R398239&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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