2-(3'-hydroxy,4'-methoxyphenylethyl)-4-methoxyq

Inchi: InChI=1S/C19H19NO3/c1-22-18-10-8-13(11-17(18)21)7-9-14-12-19(23-2)15-5-3-4-6-16(
InchiKey: UIVNIUPIHQVAQN-UHFFFAOYSA-N
Formula: C19H19NO3
SMILES: COc1ccc(CCc2cc(OC)c3ccccc3n2)cc1O
Mol. weight [g/mol]: 309.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	3.743		Crippen Method
mcvol	239.180	ml/mol	McGowan Method
rinpol	2775.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R398264&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