2,4-Dimethyl-3,5-di(4-methoxyphenyl)pyridine

Other names: 2,4-Dimethyl-3,5-di-(40-methoxyphenyl)pyridine
Inchi: InChI=1S/C21H21NO2/c1-14-20(16-5-9-18(23-3)10-6-16)13-22-15(2)21(14)17-7-11-19(2
InchiKey: OOHLKKHQGOJSQI-UHFFFAOYSA-N
Formula: C21H21NO2
SMILES: COc1ccc(-c2cnc(C)c(-c3ccc(OC)cc3)c2C)cc1
Mol. weight [g/mol]: 319.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.63		Crippen Method
logp	5.050		Crippen Method
mcvol	257.190	ml/mol	McGowan Method
rinpol	2711.00		NIST Webbook
rinpol	2711.00		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=U370396&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