

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

Other names: 2,4-Dimethyl-3,5-di-(4-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
rmpol	2711.00		NIST Webbook
rmpol	2711.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rmpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/96-218-4/2-4-Dimethyl-3-5-di-4-methoxyphenyl-pyridine.pdf>

Generated by Cheméo on 2024-05-04 15:45:33.346100845 +0000 UTC m=+17126782.266678164.

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