

2,6-Dimethyl-3,5-di(4-methoxyphenyl)pyridine

Other names:	2,6-Dimethyl-3,5-di-(4-methoxyphenyl)pyridine
Inchi:	InChI=1S/C21H21NO2/c1-14-20(16-5-9-18(23-3)10-6-16)13-21(15(2)22-14)17-7-11-19(2
InchiKey:	DXLBOCYGBZWBKW-UHFFFAOYSA-N
Formula:	C21H21NO2
SMILES:	COc1ccc(-c2cc(-c3ccc(OC)cc3)c(C)nc2C)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/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=U370395&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

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