

2,6-Pyridinedicarboxylic acid, butyl 2-methoxyphenyl ester

Inchi: InChI=1S/C18H19NO5/c1-3-4-12-23-17(20)13-8-7-9-14(19-13)18(21)24-16-11-6-5-10-15
InchiKey: HHLABJALWWGJNK-UHFFFAOYSA-N
Formula: C18H19NO5
SMILES: CCCOC(=O)c1cccc(C(=O)Oc2ccccc2OC)n1
Mol. weight [g/mol]: 329.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.94		Crippen Method
logp	3.266		Crippen Method
mcvol	247.690	ml/mol	McGowan Method
rinpola	2586.00		NIST Webbook

Sources

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=U369216&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

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