

# 2,6-Pyridinedicarboxylic acid, butyl 2-isopropoxyphenyl ester

**Inchi:** InChI=1S/C20H23NO5/c1-4-5-13-24-19(22)15-9-8-10-16(21-15)20(23)26-18-12-7-6-11-1  
**InchiKey:** YTFWMCDMBFNKII-UHFFFAOYSA-N  
**Formula:** C20H23NO5  
**SMILES:** CCCOC(=O)c1cccc(C(=O)Oc2ccccc2OC(C)C)n1  
**Mol. weight [g/mol]:** 357.40

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.89		Crippen Method
logp	4.045		Crippen Method
mcvol	275.870	ml/mol	McGowan Method
rinpola	2600.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369126&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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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