

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

Inchi:	InChI=1S/C18H19NO4/c1-3-4-12-22-17(20)14-9-7-10-15(19-14)18(21)23-16-11-6-5-8-13
InchiKey:	GAXPXEIGOQHTLU-UHFFFAOYSA-N
Formula:	C18H19NO4
SMILES:	CCCCOC(=O)c1cccc(C(=O)Oc2ccccc2C)n1
Mol. weight [g/mol]:	313.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.30		Crippen Method
logp	3.566		Crippen Method
mcvol	241.820	ml/mol	McGowan Method
rinpola	2449.00		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=U369121&Units=SI

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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