

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

Inchi:	InChI=1S/C17H17NO4/c1-3-11-21-16(19)13-8-6-9-14(18-13)17(20)22-15-10-5-4-7-12(15)
InchiKey:	UXGSVBUQCUCNEO-UHFFFAOYSA-N
Formula:	C17H17NO4
SMILES:	CCCOC(=O)c1cccc(C(=O)Oc2ccccc2C)n1
Mol. weight [g/mol]:	299.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.88		Crippen Method
logp	3.176		Crippen Method
mcvol	227.730	ml/mol	McGowan Method
rinsol	2352.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369119&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	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
rinsol:	Non-polar retention indices

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