

2,6-Pyridinedicarboxylic acid, 2-isopropoxyphenyl octyl ester

Inchi:	InChI=1S/C24H31NO5/c1-4-5-6-7-8-11-17-28-23(26)19-13-12-14-20(25-19)24(27)30-22
InchiKey:	DHGWTQMZBYUKJE-UHFFFAOYSA-N
Formula:	C24H31NO5
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2OC(C)C)n1
Mol. weight [g/mol]:	413.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.57		Crippen Method
logp	5.605		Crippen Method
mcvol	332.230	ml/mol	McGowan Method
rinpola	2970.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369128&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
rinpola:	Non-polar retention indices

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