2,6-Pyridinedicarboxylic acid, 3-methylbutyl octyl ester

Inchi: InChI=1S/C20H31NO4/c1-4-5-6-7-8-9-14-24-19(22)17-11-10-12-18(21-17)20(23)25-15-1
InchiKey: GJNXIIOHOJIBSX-UHFFFAOYSA-N
Formula: C20H31NO4
SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)C)n1
Mol. weight [g/mol]: 349.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.09		Crippen Method
logp	4.802		Crippen Method
mcvol	293.760	ml/mol	McGowan Method
rinpol	2510.00		NIST Webbook
rinpol	2510.00		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=U368320&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
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.