2,6-Pyridinedicarboxylic acid, neopentyl octyl ester

Inchi: InChI=1S/C20H31NO4/c1-5-6-7-8-9-10-14-24-18(22)16-12-11-13-17(21-16)19(23)25-15-

InchiKey: HWVDOJMPZTVMAT-UHFFFAOYSA-N

Formula: C20H31NO4

SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)(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	2416.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369004&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.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

rinpol: Non-polar retention indices