

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

Inchi:	InChI=1S/C20H31NO4/c1-4-6-7-8-9-10-14-24-19(22)17-12-11-13-18(21-17)20(23)25-15
InchiKey:	FAKRFCOKABYSRD-UHFFFAOYSA-N
Formula:	C20H31NO4
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)CC)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	2502.00		NIST Webbook
rinpol	2502.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369064&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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