

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

Inchi:	InChI=1S/C23H37NO4/c1-4-5-6-7-8-9-10-11-12-17-27-22(25)20-14-13-15-21(24-20)23(2
InchiKey:	BWUQYCJPBKOVMR-UHFFFAOYSA-N
Formula:	C23H37NO4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)C)n1
Mol. weight [g/mol]:	391.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.34		Crippen Method
logp	5.972		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
rinsol	2808.00		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=U368323&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/31-860-2/2-6-Pyridinedicarboxylic-acid-3-methylbutyl-undecyl-ester.pdf>

Generated by Cheméo on 2024-04-23 19:39:17.548835987 +0000 UTC m=+16190406.469413299.

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