

2,6-Pyridinedicarboxylic acid, dodecyl isobutyl ester

Inchi:	InChI=1S/C23H37NO4/c1-4-5-6-7-8-9-10-11-12-13-17-27-22(25)20-15-14-16-21(24-20)2
InchiKey:	LBZUIRAXRCQLIS-UHFFFAOYSA-N
Formula:	C23H37NO4
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(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
rinpola	2805.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U368858&Units=SI

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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