

2,6-Pyridinedicarboxylic acid, dodecyl isobutyl ester

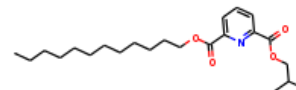
InChI: InChI=1S/C23H37NO4/c1-4-5-6-7-8-9-10-11-12-13-17-27-22(25)20-15-14-16-21(24-20)23(26)28-18-19(2)3/h14-16,19H,4-13,17-18H2,1-3H3

InChI Key: LBZUIRAXRCQLIS-UHFFFAOYSA-N

Formula: C23H37NO4

SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)C)n1

Molecular Weight: 391.54



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	5.97		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H37NO4/c1-4-5-6-7-8-9-10-11-12-13-17-27-22\(25\)20-15-14-16-21\(24-20\)23\(26\)28-18-19\(2\)3/h14-16,19H,4-13,17-18H2,1-3H3](http://webbook.nist.gov/cgi/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)23(26)28-18-19(2)3/h14-16,19H,4-13,17-18H2,1-3H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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