

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

Inchi: InChI=1S/C21H33NO4/c1-4-5-6-7-8-9-10-15-25-20(23)18-12-11-13-19(22-18)21(24)26-1
InchiKey: HXERBTXHPAZDPW-UHFFFAOYSA-N
Formula: C21H33NO4
SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)C)n1
Mol. weight [g/mol]: 363.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.50		Crippen Method
logp	5.192		Crippen Method
mcvol	307.850	ml/mol	McGowan Method
rinsol	2607.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368321&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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