

2,6-Pyridinedicarboxylic acid, ethyl 1-methoxydec-4-yl ester

Inchi: InChI=1S/C20H31NO5/c1-4-6-7-8-11-16(12-10-15-24-3)26-20(23)18-14-9-13-17(21-18)1
InchiKey: UMLMWVIEIPJQQ-UHFFFAOYSA-N
Formula: C20H31NO5
SMILES: CCCCCC(CCCOC)OC(=O)c1cccc(C(=O)OCC)n1
Mol. weight [g/mol]: 365.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.53		Crippen Method
logp	4.181		Crippen Method
mcvol	299.630	ml/mol	McGowan Method
rinpol	2509.00		NIST Webbook
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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=U369242&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
rinpol: Non-polar retention indices

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