2,6-Pyridinedicarboxylic acid, 2-ethylbutyl propyl ester

Inchi: InChI=1S/C16H23NO4/c1-4-10-20-15(18)13-8-7-9-14(17-13)16(19)21-11-12(5-2)6-3/h7-9
InchiKey: AGKVQBKIPKEIFW-UHFFFAOYSA-N
Formula: C16H23NO4
SMILES: CCCOC(=O)c1cccc(C(=O)OCC(CC)CC)n1
Mol. weight [g/mol]: 293.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.41		Crippen Method
logp	3.241		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369037&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol: Non-polar retention indices

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