

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

Inchi: InChI=1S/C20H31NO4/c1-4-7-8-9-10-14-24-19(22)17-12-11-13-18(21-17)20(23)25-15-16
InchiKey: WJSXE BMGFYLVKK-UHFFFAOYSA-N
Formula: C₂₀H₃₁NO₄
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCC(CC)CC)n1
Mol. weight [g/mol]: 349.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.09		Crippen Method
logp	4.802		Crippen Method
mcvol	293.760	ml/mol	McGowan Method
rinpol	2494.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369043&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

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