

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

Inchi: InChI=1S/C20H31NO4/c1-4-6-7-8-9-14-24-19(22)17-12-10-13-18(21-17)20(23)25-15-16
InchiKey: VMXDXTARHPPMJC-UHFFFAOYSA-N
Formula: C20H31NO4
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCC(C)CCC)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
rinpole	2486.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U369087&Units=SI>

Legend

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

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