

2,6-Pyridinedicarboxylic acid, 2-methylhex-3-yl 2-methylpentyl ester

Inchi: InChI=1S/C20H31NO4/c1-6-9-15(5)13-24-19(22)16-11-8-12-17(21-16)20(23)25-18(10-7)
InchiKey: FQDVQJCMCPGECM-UHFFFAOYSA-N
Formula: C20H31NO4
SMILES: CCCC(C)COC(=O)c1cccc(C(=O)OC(CCC)C(C)C)n1
Mol. weight [g/mol]: 349.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.96		Crippen Method
logp	4.656		Crippen Method
mcvol	293.760	ml/mol	McGowan Method
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369085&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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