

2,6-Pyridinedicarboxylic acid, isobutyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C19H29NO4/c1-13(2)11-23-17(21)15-8-7-9-16(20-15)18(22)24-12-14(3)10-19
InchiKey:	MBVJGYCPMYKJAT-UHFFFAOYSA-N
Formula:	C19H29NO4
SMILES:	CC(C)COC(=O)c1cccc(C(=O)OCC(C)CC(C)(C)C)n1
Mol. weight [g/mol]:	335.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.18		Crippen Method
logp	4.123		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
rinpole	2235.00		NIST Webbook

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=U368789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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