

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

Inchi:	InChI=1S/C20H31NO4/c1-6-10-18(14(4)5)25-20(23)17-12-9-11-16(21-17)19(22)24-13-15
InchiKey:	IRARDJZYNUJZSX-UHFFFAOYSA-N
Formula:	C20H31NO4
SMILES:	CCCC(OC(=O)c1cccc(C(=O)OCC(CC)CC)n1)C(C)C
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
rinpola	2314.00		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=U369041&Units=SI

Legend

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

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