

2,6-Pyridinedicarboxylic acid, hexadecyl 2-methylbutyl ester

Inchi:	InChI=1S/C28H47NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-22-32-27(30)25-20-19
InchiKey:	BAWHSFNCTVUFKM-UHFFFAOYSA-N
Formula:	C28H47NO4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)CC)n1
Mol. weight [g/mol]:	461.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.43		Crippen Method
logp	7.923		Crippen Method
mcvol	406.480	ml/mol	McGowan Method
rinpola	3194.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U369072&Units=SI

Legend

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

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