

2,6-Pyridinedicarboxylic acid, dodecyl 4-octyl ester

Inchi:	InChI=1S/C27H45NO4/c1-4-7-9-10-11-12-13-14-15-16-22-31-26(29)24-20-17-21-25(28-2)
InchiKey:	HDYAYVMZPNIKCF-UHFFFAOYSA-N
Formula:	C27H45NO4
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(CCC)CCCC)n1
Mol. weight [g/mol]:	447.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.37		Crippen Method
logp	7.675		Crippen Method
mcvol	392.390	ml/mol	McGowan Method
rinpole	3026.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368841&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
rinpole:	Non-polar retention indices

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