

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

Inchi:	InChI=1S/C22H35NO4/c1-4-7-9-10-11-17-26-21(24)19-15-12-16-20(23-19)22(25)27-18(
InchiKey:	OOJFLANFNSKYAG-UHFFFAOYSA-N
Formula:	C22H35NO4
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)OC(CCC)CCCC)n1
Mol. weight [g/mol]:	377.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.28		Crippen Method
logp	5.724		Crippen Method
mcvol	321.940	ml/mol	McGowan Method
rinpol	2575.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368836&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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