

2,6-Pyridinedicarboxylic acid, pentyl tridecyl ester

Inchi:	InChI=1S/C25H41NO4/c1-3-5-7-8-9-10-11-12-13-14-16-21-30-25(28)23-19-17-18-22(26)
InchiKey:	WCLMXUZVCMOHOQ-UHFFFAOYSA-N
Formula:	C25H41NO4
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCC)n1
Mol. weight [g/mol]:	419.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.42		Crippen Method
logp	6.896		Crippen Method
mcvol	364.210	ml/mol	McGowan Method
rinpol	3019.00		NIST Webbook
rinpol	3019.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368291&Units=SI
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

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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