

2,6-Pyridinedicarboxylic acid, decyl heptyl ester

Inchi:	InChI=1S/C24H39NO4/c1-3-5-7-9-10-11-13-15-20-29-24(27)22-18-16-17-21(25-22)23(20)
InchiKey:	DEHPLIBOHLQEIR-UHFFFAOYSA-N
Formula:	C24H39NO4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCC)n1
Mol. weight [g/mol]:	405.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.00		Crippen Method
logp	6.506		Crippen Method
mcvol	350.120	ml/mol	McGowan Method
rinsol	2929.00		NIST Webbook

Sources

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=U368810&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/60-053-6/2-6-Pyridinedicarboxylic-acid-decyl-heptyl-ester.pdf>

Generated by Cheméo on 2024-04-25 16:21:49.176000411 +0000 UTC m=+16351358.096577747.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.