

2,6-Pyridinedicarboxylic acid, di(2-pentyl) ester

Inchi:	InChI=1S/C17H25NO4/c1-5-8-12(3)21-16(19)14-10-7-11-15(18-14)17(20)22-13(4)9-6-2/
InchiKey:	YQTJUERTARQIW-UHFFFAOYSA-N
Formula:	C17H25NO4
SMILES:	CCCC(C)OC(=O)c1cccc(C(=O)OC(C)CCC)n1
Mol. weight [g/mol]:	307.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.29		Crippen Method
logp	3.772		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
rinpol	2062.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368349&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/29-264-7/2-6-Pyridinedicarboxylic-acid-di-2-pentyl-ester.pdf>

Generated by Cheméo on 2024-04-19 22:45:49.345027434 +0000 UTC m=+15855998.265604749.

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