

2,6-Pyridinedicarboxylic acid, heptadecyl 2-methylpentyl ester

Inchi:	InChI=1S/C30H51NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-24-34-29(32)27-22
InchiKey:	PHKWNFZVTNTDIE-UHFFFAOYSA-N
Formula:	C30H51NO4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)CCC)n1
Mol. weight [g/mol]:	489.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.27		Crippen Method
logp	8.703		Crippen Method
mcvol	434.660	ml/mol	McGowan Method
rinpola	3311.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369097&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
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/32-221-0/2-6-Pyridinedicarboxylic-acid-heptadecyl-2-methylpentyl-ester.pdf>

Generated by Cheméo on 2024-04-23 10:19:06.728995344 +0000 UTC m=+16156795.649572659.

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