

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

Inchi:	InChI=1S/C23H37NO4/c1-5-9-12-18(7-3)16-27-22(25)20-14-11-15-21(24-20)23(26)28-17
InchiKey:	UBDWUZZNIYUTOI-UHFFFAOYSA-N
Formula:	C23H37NO4
SMILES:	CCCCC(CC)COC(=O)c1cccc(C(=O)OCC(CC)CCCC)n1
Mol. weight [g/mol]:	391.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.10		Crippen Method
logp	5.828		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
rinsol	2667.00		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=U368280&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

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