

2,6-Pyridinedicarboxylic acid, butyl heptyl ester

Inchi:	InChI=1S/C18H27NO4/c1-3-5-7-8-9-14-23-18(21)16-12-10-11-15(19-16)17(20)22-13-6-4
InchiKey:	VCWXGGCOUGRULK-UHFFFAOYSA-N
Formula:	C18H27NO4
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)OCCCC)n1
Mol. weight [g/mol]:	321.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.49		Crippen Method
logp	4.166		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
rinpol	2359.00		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=U369023&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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