

2,6-Pyridinedicarboxylic acid, heptyl hexyl ester

Inchi:	InChI=1S/C20H31NO4/c1-3-5-7-9-11-16-25-20(23)18-14-12-13-17(21-18)19(22)24-15-10
InchiKey:	LAZYQTVFJGELQV-UHFFFAOYSA-N
Formula:	C20H31NO4
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)OCCCCC)n1
Mol. weight [g/mol]:	349.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.33		Crippen Method
logp	4.946		Crippen Method
mcvol	293.760	ml/mol	McGowan Method
rinpola	2550.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368776&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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