

2,6-Pyridinedicarboxylic acid, hexyl phenethyl ester

Inchi:	InChI=1S/C21H25NO4/c1-2-3-4-8-15-25-20(23)18-12-9-13-19(22-18)21(24)26-16-14-17
InchiKey:	DVCYEAVXFBCDEZ-UHFFFAOYSA-N
Formula:	C21H25NO4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)n1
Mol. weight [g/mol]:	355.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.85		Crippen Method
logp	4.218		Crippen Method
mcvol	284.090	ml/mol	McGowan Method
rinsol	2782.00		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=U369226&Units=SI

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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