

2,6-Pyridinedicarboxylic acid, pentyl phenethyl ester

Inchi: InChI=1S/C20H23NO4/c1-2-3-7-14-24-19(22)17-11-8-12-18(21-17)20(23)25-15-13-16-9
InchiKey: KENXGFRBKKNJD-UHFFFAOYSA-N
Formula: C₂₀H₂₃NO₄
SMILES: CCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)n1
Mol. weight [g/mol]: 341.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.43		Crippen Method
logp	3.828		Crippen Method
mcvol	270.000	ml/mol	McGowan Method
rinpol	2683.00		NIST Webbook
rinpol	2683.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369225&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
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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