

3-Pyridinecarboxylic acid, hexadecyl ester

Other names: Nicotinic acid, hexadecyl ester
hexadecyl nicotinate

Inchi: InChI=1S/C22H37NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-25-22(24)21-17-16-18-

InchiKey: SIYPIMGFUQHRFF-UHFFFAOYSA-N

Formula: C22H37NO2

SMILES: CCCCCCCCCCCCCCCCCOC(=O)c1cccnc1

Mol. weight [g/mol]: 347.53

CAS: 66170-39-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.76		Crippen Method
logp	6.720		Crippen Method
mcvol	314.500	ml/mol	McGowan Method
rinpol	2641.00		NIST Webbook
rinpol	2641.00		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=C66170396&Units=SI>

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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