

4-Pyridinecarboxylic acid, octadecyl ester

Other names: Isonicotinic acid, octadecyl ester
Inchi: InChI=1S/C24H41NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-27-24(26)23-18-
InchiKey: VXDJNEIVBJLMMZ-UHFFFAOYSA-N
Formula: C₂₄H₄₁NO₂
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1ccncc1
Mol. weight [g/mol]: 375.59
CAS: 103225-02-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.60		Crippen Method
logp	7.500		Crippen Method
mcvol	342.680	ml/mol	McGowan Method
rinpola	2817.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C103225021&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.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
rinpola: Non-polar retention indices

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