

Isonicotinic acid, pentadecyl ester

Inchi: InChI=1S/C21H35NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-19-24-21(23)20-15-17-22-18-
InchiKey: WARULLHSRXWCPP-UHFFFAOYSA-N
Formula: C21H35NO2
SMILES: CCCCCCCCCCCCCCOC(=O)c1ccncc1
Mol. weight [g/mol]: 333.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.34		Crippen Method
logp	6.330		Crippen Method
mcvol	300.410	ml/mol	McGowan Method
rinpol	2514.00		NIST Webbook
rinpol	2514.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299890&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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