

Isonipecotic acid, N-(octanoyl)-, decyl ester

Inchi: InChI=1S/C24H45NO3/c1-3-5-7-9-10-11-13-15-21-28-24(27)22-17-19-25(20-18-22)23(20-18-22)23(20-18-22)
InchiKey: SSTLMYJUZNALN-UHFFFAOYSA-N
Formula: C₂₄H₄₅NO₃
SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)CCCCCCC)CC1
Mol. weight [g/mol]: 395.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.73		Crippen Method
logp	6.269		Crippen Method
mcvol	357.150	ml/mol	McGowan Method
rinpol	3083.00		NIST Webbook
rinpol	3083.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361576&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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