

Isonipecotic acid, N-methoxycarbonyl-, hexadecyl ester

Inchi: InChI=1S/C24H45NO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-29-23(26)22-17-19-25
InchiKey: SYWOSVPKZUHJRJ-UHFFFAOYSA-N
Formula: C24H45NO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)OC)CC1
Mol. weight [g/mol]: 411.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.79		Crippen Method
logp	6.489		Crippen Method
mcvol	363.020	ml/mol	McGowan Method
rinpol	3190.00		NIST Webbook
rinpol	3190.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U322031&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
rinpol: Non-polar retention indices

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