

Isonipecotic acid, N-methoxycarbonyl-, dodecyl ester

Inchi: InChI=1S/C20H37NO4/c1-3-4-5-6-7-8-9-10-11-12-17-25-19(22)18-13-15-21(16-14-18)20
InchiKey: RCZSYRBCWJYIFQ-UHFFFAOYSA-N
Formula: C20H37NO4
SMILES: CCCCCCCCCCCCOC(=O)C1CCN(C(=O)OC)CC1
Mol. weight [g/mol]: 355.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.12		Crippen Method
logp	4.929		Crippen Method
mcvol	306.660	ml/mol	McGowan Method
rinpol	2625.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U322028&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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