

Isonipectic acid, N-ethoxycarbonyl-, undecyl ester

Inchi:	InChI=1S/C20H37NO4/c1-3-5-6-7-8-9-10-11-12-17-25-19(22)18-13-15-21(16-14-18)20(2
InchiKey:	NGCLMSXTTKJWOL-UHFFFAOYSA-N
Formula:	C20H37NO4
SMILES:	CCCCCCCCCOC(=O)C1CCN(C(=O)OCC)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
rinsol	2577.00		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322010&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
rinsol:	Non-polar retention indices

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