

Isonipecotic acid, N-ethoxycarbonyl-, dodecyl ester

Inchi:	InChI=1S/C21H39NO4/c1-3-5-6-7-8-9-10-11-12-13-18-26-20(23)19-14-16-22(17-15-19)2
InchiKey:	WVTALFUEVISTPB-UHFFFAOYSA-N
Formula:	C21H39NO4
SMILES:	CCCCCCCCCCCCOC(=O)C1CCN(C(=O)OCC)CC1
Mol. weight [g/mol]:	369.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.54		Crippen Method
logp	5.319		Crippen Method
mcvol	320.750	ml/mol	McGowan Method
rinpola	2682.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322011&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
rinpola:	Non-polar retention indices

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