

Isonipecotic acid, N-ethoxycarbonyl-, decyl ester

Inchi:	InChI=1S/C19H35NO4/c1-3-5-6-7-8-9-10-11-16-24-18(21)17-12-14-20(15-13-17)19(22)2
InchiKey:	JPRSAZPTNIZCKO-UHFFFAOYSA-N
Formula:	C19H35NO4
SMILES:	CCCCCCCCCOC(=O)C1CCN(C(=O)OCC)CC1
Mol. weight [g/mol]:	341.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.70		Crippen Method
logp	4.539		Crippen Method
mcvol	292.570	ml/mol	McGowan Method
rinsol	2474.00		NIST Webbook
rinsol	2474.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322009&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/27-420-5/Isonipecotic-acid-N-ethoxycarbonyl-decyl-ester.pdf>

Generated by Cheméo on 2024-04-29 23:17:22.124472495 +0000 UTC m=+16721891.045049807.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.