

Pipecolic acid, N-ethoxycarbonyl-, undecyl ester

Inchi: InChI=1S/C20H37NO4/c1-3-5-6-7-8-9-10-11-14-17-25-19(22)18-15-12-13-16-21(18)20(2)
InchiKey: YXDACQJXIVCOST-UHFFFAOYSA-N
Formula: C20H37NO4
SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)OCC
Mol. weight [g/mol]: 355.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.47		Crippen Method
logp	5.071		Crippen Method
mcvol	306.660	ml/mol	McGowan Method
rinpole	2512.00		NIST Webbook
rinpole	2512.00		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=U393077&Units=SI>

Legend

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

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