

Isonipecotic acid, N-ethoxycarbonyl-, octyl ester

Inchi: InChI=1S/C17H31NO4/c1-3-5-6-7-8-9-14-22-16(19)15-10-12-18(13-11-15)17(20)21-4-2/
InchiKey: QKZDHJOFYSFFTN-UHFFFAOYSA-N
Formula: C17H31NO4
SMILES: CCCCCCOC(=O)C1CCN(C(=O)OCC)CC1
Mol. weight [g/mol]: 313.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.86		Crippen Method
logp	3.759		Crippen Method
mcvol	264.390	ml/mol	McGowan Method
rinsol	2272.00		NIST Webbook
rinsol	2272.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U322007&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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