

Isonipecotic acid, n-butoxycarbonyl-, ethyl ester

Inchi: InChI=1S/C13H23NO4/c1-3-5-10-18-13(16)14-8-6-11(7-9-14)12(15)17-4-2/h11H,3-10H2
InchiKey: KRALZPJDIYIDNR-UHFFFAOYSA-N
Formula: C13H23NO4
SMILES: CCCCOC(=O)N1CCC(C(=O)OCC)CC1
Mol. weight [g/mol]: 257.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.19		Crippen Method
logp	2.198		Crippen Method
mcvol	208.030	ml/mol	McGowan Method
rinpol	1866.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.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=U322045&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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