

Isonipecotic acid, n-butoxycarbonyl-, hexyl ester

Inchi:	InChI=1S/C17H31NO4/c1-3-5-7-8-14-21-16(19)15-9-11-18(12-10-15)17(20)22-13-6-4-2/
InchiKey:	MRAWHIWOVCKAKQ-UHFFFAOYSA-N
Formula:	C17H31NO4
SMILES:	CCCCCOC(=O)C1CCN(C(=O)OCCCC)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
rinpola	2276.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U322051&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/93-218-7/Isonipecotic-acid-n-butoxycarbonyl-hexyl-ester.pdf>

Generated by Cheméo on 2024-04-29 05:17:34.972401449 +0000 UTC m=+16657103.892978761.

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