

Isonipecotic acid, N-isobutoxycarbonyl-, pentyl ester

Inchi:	InChI=1S/C16H29NO4/c1-4-5-6-11-20-15(18)14-7-9-17(10-8-14)16(19)21-12-13(2)3/h13
InchiKey:	PCWODTPUJVUQBH-UHFFFAOYSA-N
Formula:	C16H29NO4
SMILES:	CCCCCOC(=O)C1CCN(C(=O)OCC(C)C)CC1
Mol. weight [g/mol]:	299.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.20		Crippen Method
logp	3.224		Crippen Method
mcvol	250.300	ml/mol	McGowan Method
rinpola	2123.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322063&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/57-975-7/Isonipecotic-acid-N-isobutoxycarbonyl-pentyl-ester.pdf>

Generated by Cheméo on 2024-04-20 04:33:23.580197174 +0000 UTC m=+15876852.500774490.

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