

Isonipecotic acid, n-butoxycarbonyl-, dodecyl ester

Inchi:	InChI=1S/C23H43NO4/c1-3-5-7-8-9-10-11-12-13-14-20-27-22(25)21-15-17-24(18-16-21)
InchiKey:	VOMRZQJJFAQBQW-UHFFFAOYSA-N
Formula:	C23H43NO4
SMILES:	CCCCCCCCCCCCOC(=O)C1CCN(C(=O)OCCCC)CC1
Mol. weight [g/mol]:	397.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.38		Crippen Method
logp	6.099		Crippen Method
mcvol	348.930	ml/mol	McGowan Method
rinpol	2929.00		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=U322057&Units=SI

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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