

Isonipecotic acid, n-butoxycarbonyl-, heptyl ester

Inchi:	InChI=1S/C18H33NO4/c1-3-5-7-8-9-15-22-17(20)16-10-12-19(13-11-16)18(21)23-14-6-4
InchiKey:	CTGBRBNZIAAKMC-UHFFFAOYSA-N
Formula:	C18H33NO4
SMILES:	CCCCCCCOC(=O)C1CCN(C(=O)OCCCC)CC1
Mol. weight [g/mol]:	327.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.28		Crippen Method
logp	4.149		Crippen Method
mcvol	278.480	ml/mol	McGowan Method
rinpola	2371.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322052&Units=SI
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

Legend

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

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