

Isonipecotic acid, N-(3-methylbutyryl)-, octyl ester

Inchi:	InChI=1S/C19H35NO3/c1-4-5-6-7-8-9-14-23-19(22)17-10-12-20(13-11-17)18(21)15-16(2)
InchiKey:	OLRQVRGCJXZSGH-UHFFFAOYSA-N
Formula:	C19H35NO3
SMILES:	CCCCCCCCOC(=O)C1CCN(C(=O)CC(C)C)CC1
Mol. weight [g/mol]:	325.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.39		Crippen Method
logp	4.175		Crippen Method
mcvol	286.700	ml/mol	McGowan Method
rinpola	2497.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360992&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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