

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

Inchi:	InChI=1S/C18H33NO3/c1-4-5-6-7-8-13-22-18(21)16-9-11-19(12-10-16)17(20)14-15(2)3/
InchiKey:	MBYAKLHPYOQAGV-UHFFFAOYSA-N
Formula:	C18H33NO3
SMILES:	CCCCCCCCOC(=O)C1CCN(C(=O)CC(C)C)CC1
Mol. weight [g/mol]:	311.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	3.785		Crippen Method
mcvol	272.610	ml/mol	McGowan Method
rinpol	2392.00		NIST Webbook

Sources

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=U360991&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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