

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

Inchi:	InChI=1S/C14H25NO3/c1-4-9-18-14(17)12-5-7-15(8-6-12)13(16)10-11(2)3/h11-12H,4-10H
InchiKey:	NNZSAHPBZZGYLE-UHFFFAOYSA-N
Formula:	C14H25NO3
SMILES:	CCCOC(=O)C1CCN(C(=O)CC(C)C)CC1
Mol. weight [g/mol]:	255.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	2.224		Crippen Method
mcvol	216.250	ml/mol	McGowan Method
rinpol	1973.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U360986&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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