

# Isonipecotic acid, N-(3-methylbutyryl)-, heptadecyl ester

**Inchi:** InChI=1S/C28H53NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23-32-28(31)26-19-2  
**InchiKey:** YYCXSTIDIHYRJT-UHFFFAOYSA-N  
**Formula:** C28H53NO3  
**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)CC(C)C)CC1  
**Mol. weight [g/mol]:** 451.73

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.16		Crippen Method
logp	7.686		Crippen Method
mcvol	413.510	ml/mol	McGowan Method
rinpola	3436.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=U361001&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  
**rinpola:** Non-polar retention indices

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