

# 7-(2-Methylbutyryl)-9-echimidinylretronecine

**Inchi:** InChI=1S/C20H33NO7/c1-6-12(2)17(23)28-15-8-10-21-9-7-14(16(15)21)11-27-18(24)20  
**InchiKey:** CJYGEJQKEOQHSM-AVGQWPLZSA-N  
**Formula:** C20H33NO7  
**SMILES:** CCC(C)C(=O)OC1CCN2CC=C(COC(=O)C(O)(C(C)O)C(C)(C)O)C12  
**Mol. weight [g/mol]:** 399.48

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	0.385		Crippen Method
mcvol	309.110	ml/mol	McGowan Method
rinpol	2512.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R299573&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/65-002-7/7-2-Methylbutyryl-9-echimidinylretronecine.pdf>

Generated by Cheméo on 2024-04-16 21:20:27.903155598 +0000 UTC m=+15591676.823732913.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.