

# Isobutyric acid, 1-(diethoxyphosphinyl)-2-methylpropenyl

**Inchi:**  
**ester**

InChI=1S/C12H23O5P/c1-7-15-18(14,16-8-2)12(10(5)6)17-11(13)9(3)4/h9H,7-8H2,1-6H3

**InchiKey:**

BKDDPKBOEGBUSD-UHFFFAOYSA-N

**Formula:**

C12H23O5P

**SMILES:**

CCOP(=O)(OCC)C(OC(=O)C(C)C)=C(C)C

**Mol. weight [g/mol]:**

278.28

**CAS:**

116595-11-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.76		Crippen Method
logp	3.703		Crippen Method
mcvol	221.150	ml/mol	McGowan Method

## Sources

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C116595110&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:**

[https://www.cheméo.com/doc/models/crippen\\_log10ws](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

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