

# Phosphoric acid, 7-chlorobicyclo[3.2.0]hepta-2,6-dien-6-yl dimethyl ester

Other names: Heptenophos  
7-Chlorobicyclo[3.2.0]hepta-2,6-dien-6-yl dimethyl phosphate

Hoe 02982

Hostaquick

OMS 1845

Ragadan

**Inchi:** InChI=1S/C9H12ClO4P/c1-12-15(11,13-2)14-9-7-5-3-4-6(7)8(9)10/h3-4,6-7H,5H2,1-2H3

**InchiKey:** GBAWQJNHVWMTLU-UHFFFAOYSA-N

**Formula:** C9H12ClO4P

**SMILES:** COP(=O)(OC)OC1=C(Cl)C2C=CCC12

**Mol. weight [g/mol]:** 250.62

**CAS:** 23560-59-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	3.060		Crippen Method
mcvol	163.530	ml/mol	McGowan Method
rinpol	1541.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1539.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C23560590&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**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>

# Legend

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

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