

# Hydroxyacetic acid, pentylboronate

**Inchi:** InChI=1S/C7H13BO3/c1-2-3-4-5-8-10-6-7(9)11-8/h2-6H2,1H3  
**InchiKey:** MKVAYTRUZWMUTR-UHFFFAOYSA-N  
**Formula:** C7H13BO3  
**SMILES:** CCCCCB1OCC(=O)O1  
**Mol. weight [g/mol]:** 155.99

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.74		Crippen Method
logp	1.238		Crippen Method
rinpol	1019.00		NIST Webbook
rinpol	1018.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R62136&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  
**rinpol:** Non-polar retention indices

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<https://www.chemeo.com/cid/68-878-3/Hydroxyacetic-acid-pentylboronate.pdf>

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