

# Ethanediol, heptylboronate

**Inchi:** InChI=1S/C9H19BS2/c1-2-3-4-5-6-7-10-11-8-9-12-10/h2-9H2,1H3  
**InchiKey:** BJZKTHUUNKAXRR-UHFFFAOYSA-N  
**Formula:** C9H19BS2  
**SMILES:** CCCCCCB1SCCS1  
**Mol. weight [g/mol]:** 202.19

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -1.92   |      | Crippen Method |
| logp          | 3.925   |      | Crippen Method |
| rinpol        | 1218.00 |      | NIST Webbook   |
| rinpol        | 1214.00 |      | NIST Webbook   |

## Sources

**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)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R62104&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**rinpol:** Non-polar retention indices

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