2(?)-Hydroxybutanoic acid, pentylboronate

Inchi: InChI=1S/C9H17BO3/c1-3-5-6-7-10-12-8(4-2)9(11)13-10/h8H,3-7H2,1-2H3
InchiKey: YITORRQAYXWUFF-UHFFFAOYSA-N
Formula: C9H17BO3
SMILES: CCCCCB1OC(=O)C(CC)O1
Mol. weight [g/mol]: 184.04

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.21		Crippen Method
logp	2.017		Crippen Method
rinpol	1210.00		NIST Webbook
rinpol	1217.00		NIST Webbook
rinpol	1210.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R61992&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