

2(?)-Hydroxypropanoic acid, pentylboronate

Inchi: InChI=1S/C8H15BO3/c1-3-4-5-6-9-11-7(2)8(10)12-9/h7H,3-6H2,1-2H3
InchiKey: DIKOJYMSNFISHX-UHFFFAOYSA-N
Formula: C8H15BO3
SMILES: CCCCCB1OC(=O)C(C)O1
Mol. weight [g/mol]: 170.01

Physical Properties

Property code	Value	Unit	Source
log10ws	0.20		Crippen Method
logp	1.627		Crippen Method
rinpol	1124.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1124.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R62015&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/19-187-4/2-Hydroxypropanoic-acid-pentylboronate.pdf>

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