

2(?)-Hydroxypropanoic acid, isopentylboronate

Inchi:	InChI=1S/C8H15BO3/c1-6(2)4-5-9-11-7(3)8(10)12-9/h6-7H,4-5H2,1-3H3
InchiKey:	NTKXULUAHSUJQD-UHFFFAOYSA-N
Formula:	C8H15BO3
SMILES:	CC(C)CCB1OC(=O)C(C)O1
Mol. weight [g/mol]:	170.01

Physical Properties

Property code	Value	Unit	Source
log10ws	0.45		Crippen Method
logp	1.483		Crippen Method
rinpol	1044.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R62001&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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<https://www.chemeo.com/cid/51-848-4/2-Hydroxypropanoic-acid-isopentylboronate.pdf>

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