

# Prostaglandine F3A, benzeneboronate

**Inchi:** InChI=1S/C26H35BO5/c1-2-3-7-14-21(28)17-18-23-22(15-10-4-5-11-16-26(29)30)24-19-  
**InchiKey:** ZIIQLMHUYXHYFY-MJJIFDGMSA-N  
**Formula:** C26H35BO5  
**SMILES:** CCC=CCC(O)C=CC1C2CC(OB(c3ccccc3)O2)C1CC=CCCCC(=O)O  
**Mol. weight [g/mol]:** 438.36

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.19		Crippen Method
logp	4.277		Crippen Method
rinpol	3180.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R102122&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/61-789-9/Prostaglandine-F3A-benzeneboronate.pdf>

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