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
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