Prostaglandine F1A, methaneboronate

Inchi: InChI=1S/C21H37BO5/c1-3-4-7-10-16(23)13-14-18-17(11-8-5-6-9-12-21(24)25)19-15-20
InchiKey: IDNWUJTXIWDSGF-DEPYJBECSA-N
Formula: C21H37BO5
SMILES: CCCCCC(O)C=CC1C2CC(OB(C)O2)C1CCCCCCC(=O)O
Mol. weight [g/mol]: 380.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	4.447		Crippen Method
rinpol	2625.00		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=R102073&Units=SI

Legend

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