Prostaglandine F1A, butaneboronate

Inchi: InChI=1S/C24H43BO5/c1-3-5-9-12-19(26)15-16-21-20(13-10-7-8-11-14-24(27)28)22-18-
InchiKey: JVRQPYYICMNSEK-SAKNCAIISA-N
Formula: C24H43BO5
SMILES: CCCCCC(O)C=CC1C2CC(OB(CCCC)O2)C1CCCCCCC(=O)O
Mol. weight [g/mol]: 422.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.57		Crippen Method
logp	5.617		Crippen Method
rinpol	2885.00		NIST Webbook
rinpol	2885.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R102053&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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