

Prostaglandine F3A, methaneboronate

Inchi: InChI=1S/C21H33BO5/c1-3-4-7-10-16(23)13-14-18-17(11-8-5-6-9-12-21(24)25)19-15-20
InchiKey: BICGGUYEAFOXKO-YIWXZHFNSA-N
Formula: C21H33BO5
SMILES: CCC=CCC(O)C=CC1C2CC(OB(C)O2)C1CC=CCCCC(=O)O
Mol. weight [g/mol]: 376.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.02		Crippen Method
logp	3.999		Crippen Method
rinpol	2590.00		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=R102157&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/58-067-4/Prostaglandine-F3A-methaneboronate.pdf>

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