

Prostaglandine F3A, cyclohexaneboronate

Inchi: InChI=1S/C26H41BO5/c1-2-3-7-14-21(28)17-18-23-22(15-10-4-5-11-16-26(29)30)24-19-
InchiKey: JOUDZIRNFSJFAW-MJJIFDGMSA-N
Formula: C26H41BO5
SMILES: CCC=CCC(O)C=CC1C2CC(OB(C3CCCCC3)O2)C1CC=CCCCC(=O)O
Mol. weight [g/mol]: 444.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.01		Crippen Method
logp	5.704		Crippen Method
rinpol	3120.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R102142&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/15-694-5/Prostaglandine-F3A-cyclohexaneboronate.pdf>

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