

Prostaglandine F1A, benzeneboronate

Inchi: InChI=1S/C26H39BO5/c1-2-3-7-14-21(28)17-18-23-22(15-10-4-5-11-16-26(29)30)24-19-
InchiKey: XXGMLAHJANWBSW-ZLJGZYERSA-N
Formula: C26H39BO5
SMILES: CCCCCC(O)C=CC1C2CC(OB(c3ccccc3)O2)C1CCCCCCC(=O)O
Mol. weight [g/mol]: 442.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.49		Crippen Method
logp	4.725		Crippen Method
rinpol	3230.00		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=R102048&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/57-216-9/Prostaglandine-F1A-benzeneboronate.pdf>

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