

Prostaglandine F2A, benzeneboronate

Inchi: InChI=1S/C26H37BO5/c1-2-3-7-14-21(28)17-18-23-22(15-10-4-5-11-16-26(29)30)24-19-
InchiKey: UIUUQAIFAVANDP-HGRSCLMDSA-N
Formula: C26H37BO5
SMILES: CCCCC(O)C=CC1C2CC(OB(c3ccccc3)O2)C1CC=CCCC(=O)O
Mol. weight [g/mol]: 440.38

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -8.34 | | Crippen Method |
| logp | 4.501 | | Crippen Method |
| rinpol | 3185.00 | | 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=R102088&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/60-538-8/Prostaglandine-F2A-benzeneboronate.pdf>

Generated by Cheméo on 2024-04-18 06:13:23.024345211 +0000 UTC m=+15710051.944922526.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.