

Thromboxane B2, 9,12-methaneboronate-TMS

Inchi: InChI=1S/C21H35BO6/c1-3-4-7-10-17-13-14-20(28-22(2)27-17)18(19(24)15-16-23)11-8-
InchiKey: KMJMMFNKWSHPBV-UYURBRBMSA-N
Formula: C21H35BO6
SMILES: CCCCCC1C=CC(C(CC=CCCCC(=O)O)C(O)CC=O)OB(C)O1
Mol. weight [g/mol]: 394.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	3.792		Crippen Method
rinpol	2670.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R526513&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

Latest version available from:

<https://www.chemeo.com/cid/64-480-8/Thromboxane-B2-9-12-methaneboronate-TMS.pdf>

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