

Thromboxane B2, 9,12-butaneboronate-TMS

Inchi: InChI=1S/C24H41BO6/c1-3-5-9-12-20-15-16-23(31-25(30-20)18-6-4-2)21(22(27)17-19-2
InchiKey: DQEPUJYTFISNPI-WIUCMEPOSA-N
Formula: C24H41BO6
SMILES: CCCCCC1C=CC(C(CC=CCCCC(=O)O)C(O)CC=O)OB(CCCC)O1
Mol. weight [g/mol]: 436.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.05		Crippen Method
logp	4.962		Crippen Method
rinpol	2900.00		NIST Webbook
rinpol	2900.00		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=R526508&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/95-682-0/Thromboxane-B2-9-12-butaneboronate-TMS.pdf>

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