Ceramide 18:1/18:0 methaneboronate

Inchi: InChI=1S/C37H72BNO3/c1-4-6-8-10-12-14-16-18-19-21-23-25-27-29-31-33-37(40)39-35
InchiKey: DTUBUQCUNVSSIS-CANHMZCPSA-N
Formula: C37H72BNO3
SMILES: CCCCCCCCCCCCCC=CC1OB(C)OCC1NC(=O)CCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 589.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.09		Crippen Method
logp	11.523		Crippen Method
rinpol	4113.00		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=R385634&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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https://www.chemeo.com/cid/61-707-9/Ceramide-18-1-18-0-methaneboronate.pdf
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