

Ceramide 20:1/18:0 methaneboronate

Inchi: InChI=1S/C39H76BNO3/c1-4-6-8-10-12-14-16-18-20-22-24-26-28-30-32-34-38-37(36-43)
InchiKey: CUJRGZJAVRCMRA-AOVPEFBKSA-N
Formula: C39H76BNO3
SMILES: CCCCCCCCCCCCCC=CC1OB(C)OCC1NC(=O)CCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 617.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.93		Crippen Method
logp	12.304		Crippen Method
rinpol	4309.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R385674&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/12-781-1/Ceramide-20-1-18-0-methaneboronate.pdf>

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