Ceramide 18:1/16:0 methaneboronate

Inchi: InChI=1S/C35H68BNO3/c1-4-6-8-10-12-14-16-18-20-22-24-26-28-30-34-33(32-39-36(3)
InchiKey: VZQCMUJFAGPLPV-JODYPZOSSA-N
Formula: C35H68BNO3
SMILES: CCCCCCCCCCCCCC=CC1OB(C)OCC1NC(=O)CCCCCCCCCCCCCCC
Mol. weight [g/mol]: 561.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.25		Crippen Method
logp	10.743		Crippen Method
rinpol	3909.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R385629&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