

Ceramide 18:1/24:0 methaneboronate

Inchi: InChI=1S/C43H84BNO3/c1-4-6-8-10-12-14-16-18-19-20-21-22-23-24-25-27-29-31-33-35
InchiKey: FAELVBRVAFADJZ-GBKKFVGOSA-N
Formula: C43H84BNO3
SMILES: CCCCCCCCCCCCCC=CC1OB(C)OCC1NC(=O)CCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 673.94

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.60		Crippen Method
logp	13.864		Crippen Method
rinpol	4708.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R385654&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/57-871-2/Ceramide-18-1-24-0-methaneboronate.pdf>

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