Glycerol 1-octadecenoate, methylboronate

Inchi: InChI=1S/C22H41BO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22(24)25-19-21-20
InchiKey: AZZHEZQDSPJITC-KHPPLWFESA-N
Formula: C22H41BO4
SMILES: CCCCCCCCC=CCCCCCCCC(=O)OCC1COB(C)O1
Mol. weight [g/mol]: 380.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.60		Crippen Method
logp	6.101		Crippen Method
rinpol	2552.00		NIST Webbook
rinpol	2552.00		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=R385723&Units=SI

Legend

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