

Glycerol 1-octadecanoate, methylboronate

Inchi: InChI=1S/C22H43BO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22(24)25-19-21-20
InchiKey: NXFUDMPHYMAZKB-UHFFFAOYSA-N
Formula: C22H43BO4
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCC1COB(C)O1
Mol. weight [g/mol]: 382.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Crippen Method
logp	6.325		Crippen Method
rinpol	2572.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R385718&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/51-601-7/Glycerol-1-octadecanoate-methylboronate.pdf>

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