

Glycerol 1-hexadecanoate, methylboronate

Inchi: InChI=1S/C20H39BO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20(22)23-17-19-18-24-21
InchiKey: HMBFSXMAHIHCAL-UHFFFAOYSA-N
Formula: C20H39BO4
SMILES: CCCCCCCCCCCCCC(=O)OCC1COB(C)O1
Mol. weight [g/mol]: 354.33

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -3.91 | | Crippen Method |
| logp | 5.544 | | Crippen Method |
| rinpol | 2373.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R385694&Units=SI>

Legend

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

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