

Glycerol, 1-caproate-3-arachidate-, 2-OTMS-

Inchi: InChI=1S/C32H64O5Si/c1-6-8-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-27-32(34)
InchiKey: KCZMCDUNTUKWKE-UHFFFAOYSA-N
Formula: C32H64O5Si
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCC(COC(=O)CCCC)O[Si](C)(C)C
Mol. weight [g/mol]: 556.93

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -8.19 | | Crippen Method |
| logp | 9.915 | | Crippen Method |
| rinpol | 3355.00 | | NIST Webbook |
| rinpol | 3355.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R517089&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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.chemeo.com/cid/86-214-9/Glycerol-1-caproate-3-arachidate-2-OTMS.pdf>

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