

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

Inchi: InChI=1S/C22H44O5Si/c1-6-8-10-11-12-13-15-17-22(24)26-19-20(27-28(3,4)5)18-25-21
InchiKey: FDQGGFJNQFONII-UHFFFAOYSA-N
Formula: C22H44O5Si
SMILES: CCCCCCCCC(=O)OCC(COC(=O)CCCC)O[Si](C)(C)C
Mol. weight [g/mol]: 416.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	6.014		Crippen Method
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook

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=R517094&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/68-268-0/Glycerol-1-caproate-3-caprylate-2-OTMS.pdf>

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