

Glycerol, 1-iso-C15, 2-iso-C15, TMS

Inchi: InChI=1S/C36H72O5Si/c1-32(2)26-22-18-14-10-8-12-16-20-24-28-35(37)39-30-34(31-40)
InchiKey: HGCKCZVUBFGYGD-UHFFFAOYSA-N
Formula: C36H72O5Si
SMILES: CC(C)CCCCCCCCCCCC(=O)OCC(CO[Si](C)(C)C)OC(=O)CCCCCCCCCCCC(C)C
Mol. weight [g/mol]: 613.04

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.38		Crippen Method
logp	11.187		Crippen Method
rinpol	3461.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R398571&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/119-868-7/Glycerol-1-iso-C15-2-iso-C15-TMS.pdf>

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