3«alpha»,7«beta»,14«alpha»-trihydroxy-5«beta»-c acid, TMS

Inchi: InChI=1S/C36H72O5Si4/c1-26(16-17-32(37)40-44(10,11)12)29-20-23-36(41-45(13,14)15

InchiKey: FXIHTYHJAIHHNY-TVIBPRCASA-N

Formula: C36H72O5Si4

SMILES: CC(CCC(=O)O[Si](C)(C)C)C1CCC2(O[Si](C)(C)C)C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C

Mol. weight [g/mol]: 697.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.44		Crippen Method
logp	10.464		Crippen Method
rinpol	3184.00		NIST Webbook
rinpol	3188.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R279935&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/30-484-1/3-alpha-7-beta-14-alpha-trihydroxy-5-beta-cholan-24-oic-acid-TMS.pdf

Generated by Cheméo on 2024-10-12 03:02:02.362038799 +0000 UTC m=+3282984.999008047.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.