

# 3«alpha»,7«beta»,17«alpha»-trihydroxy-5«beta»-cholanic acid, DMESI

Inchi: nChI=1S/C40H80O5Si4/c1-16-46(8,9)42-32-22-25-38(6)31(28-32)29-35(43-47(10,11)17-19)44-20-21-23-24-33-34-36-37-39-40-41-45-48-49-50-51-52-53-54-55-56-57-58-59-60  
InchiKey: OBJAMDYRFFJLHC-GAFRAGQESA-N

Formula: C40H80O5Si4  
SMILES: CC[Si](C)(C)OC(=O)CCC(C)C1(O[Si](C)(C)CC)CCC2C3C(O[Si](C)(C)CC)CC4CC(O[Si](C)(C)CC)C5C6C7C8C9C10C11C12C13C14C15C16C17C18C19C20C21C22C23C24C25C26C27C28C29C30C31C32C33C34C35C36C37C38C39C40  
Mol. weight [g/mol]: 753.40

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	12.024		Crippen Method
rinpol	3620.00		NIST Webbook

## Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
Crippen Method: [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)  
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R279940&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.cheméo.com/cid/14-959-2/3-alpha-7-beta-17-alpha-trihydroxy-5-beta-cholan-24-oic-acid-DMESI.pdf>

Generated by Cheméo on 2024-04-18 07:50:40.624279833 +0000 UTC m=+15715889.544857149.

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