

5«alpha»-cholestan-3«beta»,17«alpha»,25-triol,

DMESI

InchiKey:

InChI=1S/C39H78O3Si3/c1-15-43(9,10)40-32-22-26-37(7)31(29-32)20-21-33-34(37)23-2

HYFKPTTUJXPZQJ-SUHCAMORSA-N

Formula:

C39H78O3Si3

SMILES:

CC[Si](C)(C)OC1CCC2(C)C(CCC3C2CCC2(C)C3CCC2(O[Si](C)(C)CC)C(C)CCCC(C)(C

Mol. weight [g/mol]:

679.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.78		Crippen Method
logp	12.446		Crippen Method
rinpol	3853.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R280009&Units=SI>

Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

rinpol:

Non-polar retention indices

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