

24-Nor-5«beta»-cholane-3«alpha»,7«alpha»,23-triol-TMS

TMS

InChI=1S/C32H64O3Si3/c1-23(17-20-33-36(4,5)6)26-13-14-27-30-28(16-19-32(26,27)3)

InchiKey:

YJQWABBWPCYXJD-PRYZTBJMSA-N

Formula:

C32H64O3Si3

SMILES:

CC(CCO[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC

Mol. weight [g/mol]:

581.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Crippen Method
logp	9.573		Crippen Method
rinpol	3199.00		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=R271293&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/20-826-2/24-Nor-5-beta-cholane-3-alpha-7-alpha-23-triol-TMS.pdf>

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