5«beta»-Cholane-3«alpha»,7«alpha»,24-triol, TMS

Inchi: InChI=1S/C33H66O3Si3/c1-24(14-13-21-34-37(4,5)6)27-15-16-28-31-29(18-20-33(27,28
InchiKey: DIDRNKWXXWKOIP-PRCCELAASA-N
Formula: C33H66O3Si3
SMILES: CC(CCCO[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC
Mol. weight [g/mol]: 595.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.73		Cheméo Relay (1.0)
logp	9.963		Crippen Method
rinpol	3298.00		NIST Webbook
tf	365.74	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R271644&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point

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