

5-«beta»-Androstan-3-«alpha»-ol-17-«beta»-carboxylate-MeTMS

InChI:
MeTMS

InChI=1S/C24H42O3Si/c1-23-13-11-17(27-28(4,5)6)15-16(23)7-8-18-19-9-10-21(22(25)26)3

InChIKey:

WGNHKXCUYIUHGD-VWACKGHCSA-N

Formula:

C24H42O3Si

SMILES:

COC(=O)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]:

406.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	6.038		Crippen Method
rinpol	2659.00		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=R393432&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/64-991-1/5-beta-Androstan-3-alpha-ol-17-beta-carboxylate-MeTMS.pdf>

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