

Castasterone, methanboronate-TMS ether

Inchi: InChI=1S/C35H65BO5Si2/c1-21(2)22(3)32(40-42(8,9)10)33(41-43(11,12)13)23(4)25-14-
InchiKey: ULTPVQNCRBQLGU-GVCKCDDBSA-N
Formula: C35H65BO5Si2
SMILES: CB1OC2CC3C(=O)CC4C(CCC5(C)C(C(C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(C)C(C)C)C
Mol. weight [g/mol]: 632.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.38		Crippen Method
logp	8.705		Crippen Method
rinpol	3617.00		NIST Webbook
rinpol	3618.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R499971&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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.chemeo.com/cid/48-827-1/Castasterone-methanboronate-TMS-ether.pdf>

Generated by Cheméo on 2024-05-03 01:33:45.47765318 +0000 UTC m=+16989274.398230495.

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