

5-Pregnene-3«beta»,20«beta»,21-triol, methylboronate-TMS

Inchi: InChI=1S/C25H43BO3Si/c1-24-13-11-18(29-30(4,5)6)15-17(24)7-8-19-20-9-10-22(23-16)
InchiKey: DYSJFFIPZVHTFM-PHLWBJBFSA-N
Formula: C25H43BO3Si
SMILES: CB1OCC(C2CCC3C4CC=C5CC(O[Si](C)(C)C)CCC5(C)C4CCC23C)O1
Mol. weight [g/mol]: 430.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Cheméo Relay (1.0)
logp	6.319		Crippen Method
rinpol	2870.00		NIST Webbook
rinpol	2870.00		NIST Webbook
tf	393.01	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R528900&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):

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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<https://www.chemeo.com/cid/123-526-1/5-Pregnene-3-beta-20-beta-21-triol-methylboronate-TMS.pdf>

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