

6-Deoxocasterone, methaneboronate

Inchi: InChI=1S/C30H52B2O4/c1-17(2)18(3)27-28(36-32(8)35-27)19(4)22-11-12-23-21-10-9-20
InchiKey: LYVSPGXNPWKSQQL-WSQGCRISA-N
Formula: C30H52B2O4
SMILES: CB1OC2CC3CCC4C(CCC5(C)C(C(C)C6OB(C)OC6C(C)C(C)C)CCC45)C3(C)CC2O1
Mol. weight [g/mol]: 498.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	6.987		Crippen Method
rinpol	3429.00		NIST Webbook
rinpol	3429.00		NIST Webbook
rinpol	3430.00		NIST Webbook
rinpol	3433.00		NIST Webbook
rinpol	3429.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R497128&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.chemeo.com/cid/118-648-2/6-Deoxocasterone-methaneboronate.pdf>

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