

Pregn-4-ene-3,20-dione, 17,21-[(methylborylene)bis(oxy)]-

Other names:

Pregn-4-ene-3,20-dione, 17,21-dihydroxy-, cyclic methaneboronate

17«alpha»,21-Dihydroxypregn-4-en-3,20-dione, 17,21-methylboronate

Inchi:

InChI=1S/C22H31BO4/c1-20-9-6-15(24)12-14(20)4-5-16-17(20)7-10-21(2)18(16)8-11-22

InchiKey:

ZGVRRSZTQWLGRB-UHFFFAOYSA-N

Formula:

C22H31BO4

SMILES:

CB1OCC(=O)C2(CCC3C4CCC5=CC(=O)CCC5(C)C4CCC32C)O1

Mol. weight [g/mol]:

370.29

CAS:

30888-52-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	3.991		Crippen Method
rinpol	2820.00		NIST Webbook
rinpol	2820.00		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=C30888529&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/95-942-1/Pregn-4-ene-3-20-dione-17-21-methylborylene-bis-oxy.pdf>

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