

Pregn-4-en-3-one, 20,21-[(methyleneborylene)bis(oxy)]-, (20R)-

Other names:

Pregn-4-en-3-one, 20«beta»,21-dihydroxy-, cyclic methanoboronate

20«beta»,21-Dihydroxypregn-4-en-3-one, 20,21-methylboronate

Inchi:

InChI=1S/C22H33BO3/c1-21-10-8-15(24)12-14(21)4-5-16-17-6-7-19(20-13-25-23(3)26-2

InchiKey:

BZHGQTRIUSTJHC-CHRBLHIJSA-N

Formula:

C22H33BO3

SMILES:

CB1OCC(C2CCC3C4CCC5=CC(=O)CCC5(C)C4CCC23C)O1

Mol. weight [g/mol]:

356.31

CAS:

30882-65-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.14		Crippen Method
logp	4.668		Crippen Method
rinpol	2850.00		NIST Webbook
rinpol	2850.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C30882656&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/84-447-3/Pregn-4-en-3-one-20-21-methyleneborylene-bis-oxy-20R.pdf>

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