

5-«beta»-Pregnan-20-one, MO

Inchi: InChI=1S/C22H37NO/c1-15(23-24-4)18-10-11-19-17-9-8-16-7-5-6-13-21(16,2)20(17)12-
InchiKey: YDHJUNUWILMLTJ-ORYYPEJMSA-N
Formula: C22H37NO
SMILES: CON=C(C)C1CCC2C3CCC4CCCCC4(C)C3CCC12C
Mol. weight [g/mol]: 331.54

Physical Properties

Property code	Value	Unit	Source
hf	-327.34	kJ/mol	Joback Method
hvap	67.65	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	6.058		Crippen Method
mcvol	288.950	ml/mol	McGowan Method
pc	1265.55	kPa	Joback Method
rinpol	2344.00		NIST Webbook
tb	836.52	K	Joback Method
tc	1078.38	K	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R486905&Units=SI>

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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