

5-Pregnen-3«beta»-ol-20-one, O-methyloxime

Other names:	5-Pregnen-3«beta»-ol-20-one, MO
Inchi:	InChI=1S/C22H35NO2/c1-14(23-25-4)18-7-8-19-17-6-5-15-13-16(24)9-11-21(15,2)20(17
InchiKey:	KKWPHPAMYMPJIV-UHFFFAOYSA-N
Formula:	C22H35NO2
SMILES:	CON=C(C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	345.52

Physical Properties

Property code	Value	Unit	Source
hf	-433.26	kJ/mol	Joback Method
hvap	85.29	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	4.949		Crippen Method
mcvol	290.520	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinpol	2681.00		NIST Webbook
tb	932.84	K	Joback Method
tc	1164.73	K	Joback Method

Sources

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=U394540&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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