

5-«beta»-Pregnan-11,20-dione, MO

Inchi: InChI=1S/C23H38N2O2/c1-15(24-26-4)18-11-12-19-17-10-9-16-8-6-7-13-22(16,2)21(17)
InchiKey: MZWPWOPEEMZKBQ-PPVJAOGMSA-N
Formula: C23H38N2O2
SMILES: CON=C(C)C1CCC2C3CCC4CCCCC4(C)C3C(=NOC)CC12C
Mol. weight [g/mol]: 374.56

Physical Properties

Property code	Value	Unit	Source
hf	-439.17	kJ/mol	Joback Method
hvap	76.43	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.670		Crippen Method
mcvol	314.590	ml/mol	McGowan Method
pc	1073.57	kPa	Joback Method
rinpol	2481.00		NIST Webbook
tb	960.98	K	Joback Method
tc	1206.29	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=R486732&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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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