

5-«alpha»-Pregnan-3,11-dione, MO

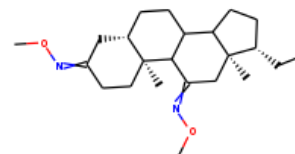
InChI: InChI=1S/C23H38N2O2/c1-6-15-8-10-19-18-9-7-16-13-17(24-26-4)11-12-22(16,2)21(18)20(25-27-5)14-23(15,19)3/h15-16,18-19,21H,6-14H2,1-5H3/b24-17+,25-20+/t15-,16-,18?,19?,21?,22-,23+/m1/s1

InChI Key: ACPIXOASZHBQJM-MXIPSPNSA-N

Formula: C₂₃H₃₈N₂O₂

SMILES: CCC1CCC2C3CCC4CC(=NOC)CCC4(C)C3C(=NOC)CC12C

Molecular Weight: 374.56



Physical Properties

Property	Value	Unit	Source
$\Delta_f H^\circ_{\text{gas}}$	-470.57	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	77.18	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	5.67		Crippen Method
P_c	1054.14	kPa	Joback Method
T_{boil}	963.58	K	Joback Method
T_c	1204.81	K	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H38N2O2/c1-6-15-8-10-19-18-9-7-16-13-17\(24-26-4\)11-12-22\(16,2\)21\(18\)20\(25-27-5\)14-23\(15,19\)3/h15-16,18-19,21H,6-14H2,1-5H3/b24-17+,25-20+/t15-,16-,18?,19?,21?,22-,23+/m1/s1](http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H38N2O2/c1-6-15-8-10-19-18-9-7-16-13-17(24-26-4)11-12-22(16,2)21(18)20(25-27-5)14-23(15,19)3/h15-16,18-19,21H,6-14H2,1-5H3/b24-17+,25-20+/t15-,16-,18?,19?,21?,22-,23+/m1/s1)

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

Legend

$\Delta_f H^\circ_{\text{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).
 T_{c} : Critical Temperature (K).

Latest version available from:

<https://www.chemeo.com/cid/19-137-9/5-%C2%ABalpha%C2%BB-Pregnan-3%2C11-dione%2C%20MO>

Generated by Cheméo on Mon, 22 Apr 2019 02:16:47 +0000.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.