# Methyl-3-oxoandrost-4-ene-17B-carboxylate, 3-MO

**Inchi:** InChI=1S/C22H33NO3/c1-21-11-9-15(23-26-4)13-14(21)5-6-16-17-7-8-19(20(24)25-3)22

**InchiKey:** SEYDYMYWIPQRHK-YRIAWWRLSA-N

**Formula:** C22H33NO3

**SMILES:** CON=C1C=C2CCC3C(CCC4(C)C(C(=O)OC)CCC34)C2(C)CC1

**Mol. weight [g/mol]:** 359.50

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -536.89 | kJ/mol | Joback Method |
| hvap | 78.82 | kJ/mol | Joback Method |
| log10ws | -5.12 | | Crippen Method |
| logp | 4.741 | | Crippen Method |
| mcvol | 292.090 | ml/mol | McGowan Method |
| pc | 1332.96 | kPa | Joback Method |
| rinpol | 2745.00 | | NIST Webbook |
| tb | 924.22 | K | Joback Method |
| tc | 1165.79 | K | Joback Method |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**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=R93163&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 |