# Yohimbine

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|---|---|
| **Other names:** | Yohimban-16-carboxylic acid, 17-hydroxy-, methyl ester, (16«alpha»,17«alpha»)- |
| | Yohimban-16«alpha»-carboxylic acid, 17«alpha»-hydroxy-, methyl ester |
| | Aphrodine |
| | Aphrosol |
| | Corynine |
| | Quebrachin |
| | Quebrachine |
| | Yohimbic acid methyl ester |
| | Yohimbin |
| | 17-Hydroxyyohimban-16-carboxylic acid methyl ester |
| | Benz[g]indolo[2,3-a]quinolizine, yohimban-16-carboxylic acid deriv. |
| | (+)-Yohimbine |
| | Yohimbol-16«alpha»-carboxylic acid, methyl ester |
| **Inchi:** | InChI=1S/C21H26N2O3/c1-26-21(25)19-15-10-17-20-14(13-4-2-3-5-16(13)22-20)8-9-23( |
| **InchiKey:** | BLGXFZZNTVWLAY-MHUZEKMJSA-N |
| **Formula:** | C21H26N2O3 |
| **SMILES:** | COC(=O)C1C(O)CCC2CN3CCc4c([nH]c5ccccc45)C3CC21 |
| **Mol. weight [g/mol]:** | 354.44 |
| **CAS:** | 146-48-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -4.09 | | Crippen Method |
| logp | 2.165 | | Crippen Method |
| mcvol | 268.520 | ml/mol | McGowan Method |
| rinpol | 3168.00 | | NIST Webbook |
| rinpol | 3130.00 | | NIST Webbook |
| rinpol | 3175.00 | | NIST Webbook |
| rinpol | 3150.00 | | NIST Webbook |

# Sources

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|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C146485&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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|---|---|
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |