# Dihydroergokryptine

**Other names:** Dihydroergocryptine
**Inchi:** InChI=1S/C32H43N5O5/c1-17(2)12-25-29(39)36-11-7-10-26(36)32(41)37(25)30(40)31(4
**InchiKey:** PBUNVLRHZGSROC-UHFFFAOYSA-N
**Formula:** C32H43N5O5
**SMILES:** CC(C)CC1C(=O)N2CCCC2C2(O)OC(NC(=O)C3CC4c5cccc6[nH]cc(c56)CC4N(C)C3)(C(
**Mol. weight [g/mol]:** 577.71
**CAS:** 76190-07-3

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -5.81 | | Crippen Method |
| logp | 2.039 | | Crippen Method |
| mcvol | 434.870 | ml/mol | McGowan Method |

# Sources

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C76190073&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# Legend

**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume