# 3'-methoxy,4'-hydroxyphenyl-ethyl)-1,2,3,4-tetrahydromethylquinoline

**Inchi:** InChI=1S/C18H21NO2/c1-21-18-12-13(7-11-17(18)20)6-9-15-10-8-14-4-2-3-5-16(14)19-

**InchiKey:** SVRGVWFUWFSROF-UHFFFAOYSA-N

**Formula:** C18H21NO2

**SMILES:** COc1cc(CCC2CCc3ccccc3N2)ccc1O

**Mol. weight [g/mol]:** 283.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 182.98 | kJ/mol | Joback Method |
| hf | -169.81 | kJ/mol | Joback Method |
| hfus | 42.28 | kJ/mol | Joback Method |
| hvap | 83.80 | kJ/mol | Joback Method |
| log10ws | -4.41 | | Crippen Method |
| logp | 3.760 | | Crippen Method |
| mcvol | 227.820 | ml/mol | McGowan Method |
| pc | 2495.01 | kPa | Joback Method |
| rinpol | 2676.00 | | NIST Webbook |
| tb | 837.16 | K | Joback Method |
| tc | 1086.83 | K | Joback Method |
| tf | 623.90 | K | Joback Method |
| vc | 0.797 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 698.67 | J/mol×K | 837.16 | Joback Method |
| cpg | 715.35 | J/mol×K | 878.77 | Joback Method |
| cpg | 730.98 | J/mol×K | 920.38 | Joback Method |
| cpg | 745.71 | J/mol×K | 961.99 | Joback Method |
| cpg | 759.67 | J/mol×K | 1003.60 | Joback Method |
| cpg | 773.01 | J/mol×K | 1045.21 | Joback Method |
| cpg | 785.85 | J/mol×K | 1086.83 | 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=R398308&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion 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 |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |