# 4-ethyl-2,5-dimethoxy-«beta»-phenethylamine-M, (HO-desamino-COOH), isomer 2, methyl-acetylated

**Inchi:** InChI=1S/C15H20O6/c1-6-11-12(18-3)7-10(8-13(17)19-4)14(20-5)15(11)21-9(2)16/h7H,6

**InchiKey:** AIUASVJFWJVONJ-UHFFFAOYSA-N

**Formula:** C15H20O6

**SMILES:** CCc1c(OC)cc(CC(=O)OC)c(OC)c1OC(C)=O

**Mol. weight [g/mol]:** 296.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -528.53 | kJ/mol | Joback Method |
| hf | -916.32 | kJ/mol | Joback Method |
| hfus | 35.04 | kJ/mol | Joback Method |
| hvap | 77.04 | kJ/mol | Joback Method |
| log10ws | -2.91 | | Crippen Method |
| logp | 1.907 | | Crippen Method |
| mcvol | 225.070 | ml/mol | McGowan Method |
| pc | 1843.58 | kPa | Joback Method |
| rinpol | 2150.00 | | NIST Webbook |
| rinpol | 2150.00 | | NIST Webbook |
| tb | 786.62 | K | Joback Method |
| tc | 990.81 | K | Joback Method |
| tf | 524.09 | K | Joback Method |
| vc | 0.852 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 645.26 | J/mol×K | 786.62 | Joback Method |
| cpg | 703.96 | J/mol×K | 956.78 | Joback Method |
| cpg | 694.34 | J/mol×K | 922.75 | Joback Method |
| cpg | 683.63 | J/mol×K | 888.72 | Joback Method |
| cpg | 671.85 | J/mol×K | 854.68 | Joback Method |
| cpg | 659.05 | J/mol×K | 820.65 | Joback Method |
| cpg | 712.45 | J/mol×K | 990.81 | Joback Method |
| dvisc | 0.0000631 | Pa×s | 786.62 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000763 | Pa×s | 742.87 | Joback Method |
| dvisc | 0.0000944 | Pa×s | 699.11 | Joback Method |
| dvisc | 0.0001202 | Pa×s | 655.36 | Joback Method |
| dvisc | 0.0001585 | Pa×s | 611.60 | Joback Method |
| dvisc | 0.0002181 | Pa×s | 567.85 | Joback Method |
| dvisc | 0.0003164 | Pa×s | 524.09 | 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=R514233&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |