# Benzeneethanamine, 2,5-dimethoxy-«alpha»,4-dimethyl-

**Other names:** Phenethylamine, 2,5-dimethoxy-«alpha»,4-dimethyl-
DOM
STP
2,5-Dimethoxy-«alpha»,4-dimethylphenylethylamine
2,5-Dimethoxy-4-methylamphetamine
2,5-Dimethoxy-4-methylphenylisopropylamine
2,5-Dimethoxymethylamphetamine
2',5'-Dimethoxy-4'-methylamphetamine
4-Methyl-2,5-dimethoxyamphetamine
(.+/-.)-1-(2,5-Dimethoxy-4-methylphenyl)-2-aminopropane
(.+/-.)-1-(4-Methyl-2,5-dimethoxyphenyl)-2-aminopropane
(.+/-.)-2,5-Dimethoxy-4-methylamphetamine
(.+/-.)-DOM
(RS)-DOM
dl-2,5-Dimethoxy-4-methylamphetamine
dl-4-Methyl-2,5-dimethoxyamphetamine
STP (hallucinogen)

**Inchi:** InChI=1S/C12H19NO2/c1-8-5-12(15-4)10(6-9(2)13)7-11(8)14-3/h5,7,9H,6,13H2,1-4H3

**InchiKey:** NTJQREUGJKIARY-UHFFFAOYSA-N

**Formula:** $C_{12}H_{19}NO_2$

**SMILES:** COc1cc(CC(C)N)c(OC)cc1C

**Mol. weight [g/mol]:** 209.28

**CAS:** 15588-95-1

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -12.31 | kJ/mol | Joback Method |
| hf | -324.82 | kJ/mol | Joback Method |
| hfus | 23.76 | kJ/mol | Joback Method |
| hvap | 61.64 | kJ/mol | Joback Method |
| log10ws | -2.95 | | Crippen Method |
| logp | 1.902 | | Crippen Method |
| mcvol | 177.900 | ml/mol | McGowan Method |
| pc | 2372.59 | kPa | Joback Method |
| rinpol | 1616.00 | | NIST Webbook |
| rinpol | 1620.00 | | NIST Webbook |
| rinpol | 1605.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 1606.00 | | NIST Webbook |
| rinpol | 1635.00 | | NIST Webbook |
| rinpol | 1616.00 | | NIST Webbook |
| rinpol | 1620.00 | | NIST Webbook |
| tb | 632.51 | K | Joback Method |
| tc | 843.83 | K | Joback Method |
| tf | 401.70 | K | Joback Method |
| vc | 0.658 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 462.71 | J/mol×K | 632.51 | Joback Method |
| cpg | 478.13 | J/mol×K | 667.73 | Joback Method |
| cpg | 492.76 | J/mol×K | 702.95 | Joback Method |
| cpg | 506.60 | J/mol×K | 738.17 | Joback Method |
| cpg | 519.65 | J/mol×K | 773.39 | Joback Method |
| cpg | 531.90 | J/mol×K | 808.61 | Joback Method |
| cpg | 543.34 | J/mol×K | 843.83 | Joback Method |

# Sources

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|---|---|
| **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=C15588951&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |

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