# 3,5-Dimethoxyphenethylamine

**Other names:** Benzeneethanamine, 3,5-dimethoxy-
**Inchi:** InChI=1S/C10H15NO2/c1-12-9-5-8(3-4-11)6-10(7-9)13-2/h5-7H,3-4,11H2,1-2H3
**InchiKey:** ZHSFEDDRTVLPHH-UHFFFAOYSA-N
**Formula:** C10H15NO2
**SMILES:** COc1cc(CCN)cc(OC)c1
**Mol. weight [g/mol]:** 181.23
**CAS:** 3213-28-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -17.08 | kJ/mol | Joback Method |
| hf | -266.79 | kJ/mol | Joback Method |
| hfus | 22.49 | kJ/mol | Joback Method |
| hvap | 56.92 | kJ/mol | Joback Method |
| log10ws | -1.95 | | Crippen Method |
| logp | 1.205 | | Crippen Method |
| mcvol | 149.720 | ml/mol | McGowan Method |
| pc | 2909.25 | kPa | Joback Method |
| tb | 582.21 | K | Joback Method |
| tc | 795.30 | K | Joback Method |
| tf | 381.64 | K | Joback Method |
| vc | 0.552 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 364.65 | J/mol×K | 582.21 | Joback Method |
| cpg | 378.45 | J/mol×K | 617.72 | Joback Method |
| cpg | 391.58 | J/mol×K | 653.24 | Joback Method |
| cpg | 404.04 | J/mol×K | 688.75 | Joback Method |
| cpg | 415.81 | J/mol×K | 724.27 | Joback Method |
| cpg | 426.90 | J/mol×K | 759.78 | Joback Method |
| cpg | 437.30 | J/mol×K | 795.30 | Joback Method |

# Sources

| | |
|---|---|
| **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=C3213283&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |