# Propanamide, N-(2,5-dimethoxyphenyl)-3-phenyl-

**Inchi:** InChI=1S/C17H19NO3/c1-20-14-9-10-16(21-2)15(12-14)18-17(19)11-8-13-6-4-3-5-7-13/h
**InchiKey:** LFAIOQIJRNRAIK-UHFFFAOYSA-N
**Formula:** C17H19NO3
**SMILES:** COc1ccc(OC)c(NC(=O)CCc2ccccc2)c1
**Mol. weight [g/mol]:** 285.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 48.29 | kJ/mol | Joback Method |
| hf | -267.64 | kJ/mol | Joback Method |
| hfus | 36.16 | kJ/mol | Joback Method |
| hvap | 77.31 | kJ/mol | Joback Method |
| log10ws | -3.95 | | Crippen Method |
| logp | 3.275 | | Crippen Method |
| mcvol | 226.160 | ml/mol | McGowan Method |
| pc | 2111.94 | kPa | Joback Method |
| rinpol | 2454.00 | | NIST Webbook |
| rinpol | 2454.00 | | NIST Webbook |
| tb | 800.56 | K | Joback Method |
| tc | 1026.74 | K | Joback Method |
| tf | 506.28 | K | Joback Method |
| vc | 0.849 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 651.94 | J/mol×K | 800.56 | Joback Method |
| cpg | 666.61 | J/mol×K | 838.26 | Joback Method |
| cpg | 680.07 | J/mol×K | 875.95 | Joback Method |
| cpg | 692.34 | J/mol×K | 913.65 | Joback Method |
| cpg | 703.46 | J/mol×K | 951.35 | Joback Method |
| cpg | 713.46 | J/mol×K | 989.04 | Joback Method |
| cpg | 722.35 | J/mol×K | 1026.74 | Joback Method |

# Sources

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|---|---|
| **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=U308119&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |