# Benzamide, 3,4-dimethoxy-N-heptyl-

**Inchi:** InChI=1S/C16H25NO3/c1-4-5-6-7-8-11-17-16(18)13-9-10-14(19-2)15(12-13)20-3/h9-10,1
**InchiKey:** UHGARZJDPDXZFM-UHFFFAOYSA-N
**Formula:** C16H25NO3
**SMILES:** CCCCCCCNC(=O)c1ccc(OC)c(OC)c1
**Mol. weight [g/mol]:** 279.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -72.54 | kJ/mol | Joback Method |
| hf | -483.53 | kJ/mol | Joback Method |
| hfus | 39.53 | kJ/mol | Joback Method |
| hvap | 72.81 | kJ/mol | Joback Method |
| log10ws | -4.57 | | Crippen Method |
| logp | 3.404 | | Crippen Method |
| mcvol | 235.830 | ml/mol | McGowan Method |
| pc | 1720.31 | kPa | Joback Method |
| rinpol | 2461.00 | | NIST Webbook |
| rinpol | 2461.00 | | NIST Webbook |
| tb | 751.00 | K | Joback Method |
| tc | 948.50 | K | Joback Method |
| tf | 468.59 | K | Joback Method |
| vc | 0.900 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 685.95 | J/mol×K | 751.00 | Joback Method |
| cpg | 701.87 | J/mol×K | 783.92 | Joback Method |
| cpg | 716.83 | J/mol×K | 816.83 | Joback Method |
| cpg | 730.85 | J/mol×K | 849.75 | Joback Method |
| cpg | 743.93 | J/mol×K | 882.66 | Joback Method |
| cpg | 756.08 | J/mol×K | 915.58 | Joback Method |
| cpg | 767.32 | J/mol×K | 948.50 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U408008&Units=SI |
| **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 |

# Legend

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|---|---|
| **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 |