# Benzoylglycylglycine

**Other names:** Glycine, N-(N-benzoylglycyl)-
Glycine, N-hippuroyl-
Hippurylglycine
**Inchi:** InChI=1S/C11H12N2O4/c14-9(12-7-10(15)16)6-13-11(17)8-4-2-1-3-5-8/h1-5H,6-7H2,(H,
**InchiKey:** FWYPSSZPXQVFRB-UHFFFAOYSA-N
**Formula:** C11H12N2O4
**SMILES:** O=C(O)CNC(=O)CNC(=O)c1ccccc1
**Mol. weight [g/mol]:** 236.22
**CAS:** 1145-32-0

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -5210.70 ± 1.40 | kJ/mol | NIST Webbook |
| gf | -190.65 | kJ/mol | Joback Method |
| hf | -416.87 | kJ/mol | Joback Method |
| hfs | -833.00 ± 1.50 | kJ/mol | NIST Webbook |
| hfus | 37.37 | kJ/mol | Joback Method |
| hvap | 92.14 | kJ/mol | Joback Method |
| log10ws | -1.14 | | Crippen Method |
| logp | -0.383 | | Crippen Method |
| mcvol | 172.630 | ml/mol | McGowan Method |
| pc | 3736.23 | kPa | Joback Method |
| ss | 314.60 | J/mol×K | NIST Webbook |
| tb | 831.89 | K | Joback Method |
| tc | 1044.36 | K | Joback Method |
| tf | 556.08 | K | Joback Method |
| vc | 0.650 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 492.96 | J/mol×K | 831.89 | Joback Method |
| cpg | 501.59 | J/mol×K | 867.30 | Joback Method |
| cpg | 509.50 | J/mol×K | 902.71 | Joback Method |

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|---|---|---|---|---|
| cpg | 516.72 | J/mol×K | 938.12 | Joback Method |
| cpg | 523.30 | J/mol×K | 973.53 | Joback Method |
| cpg | 529.26 | J/mol×K | 1008.95 | Joback Method |
| cpg | 534.66 | J/mol×K | 1044.36 | Joback Method |
| cps | 277.52 | J/mol×K | 296.70 | NIST Webbook |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1145320&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

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **cps:** | Solid phase heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase 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 |
| **ss:** | Solid phase molar entropy at standard conditions |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |