# Hippuric acid N,O-d-methyl derivative

**Other names:** Hippuric acid di-methyl derivative
**Inchi:** InChI=1S/C11H13NO3/c1-12(8-10(13)15-2)11(14)9-6-4-3-5-7-9/h3-7H,8H2,1-2H3
**InchiKey:** VJKASHDUZIYFTQ-UHFFFAOYSA-N
**Formula:** C11H13NO3
**SMILES:** COC(=O)CN(C)C(=O)c1ccccc1
**Mol. weight [g/mol]:** 207.23
**CAS:** 71533-21-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -97.91 | kJ/mol | Joback Method |
| hf | -323.69 | kJ/mol | Joback Method |
| hfus | 25.69 | kJ/mol | Joback Method |
| hvap | 60.30 | kJ/mol | Joback Method |
| log10ws | -1.32 | | Crippen Method |
| logp | 0.932 | | Crippen Method |
| mcvol | 161.080 | ml/mol | McGowan Method |
| pc | 2966.57 | kPa | Joback Method |
| rinpol | 1614.00 | | NIST Webbook |
| tb | 620.36 | K | Joback Method |
| tc | 834.16 | K | Joback Method |
| tf | 394.71 | K | Joback Method |
| vc | 0.592 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 399.97 | J/mol×K | 620.36 | Joback Method |
| cpg | 413.56 | J/mol×K | 655.99 | Joback Method |
| cpg | 426.24 | J/mol×K | 691.63 | Joback Method |
| cpg | 438.06 | J/mol×K | 727.26 | Joback Method |
| cpg | 449.03 | J/mol×K | 762.90 | Joback Method |
| cpg | 459.20 | J/mol×K | 798.53 | Joback Method |
| cpg | 468.58 | J/mol×K | 834.16 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C71533216&Units=SI |

# 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 |