# PROPANAMIDE, 2-METHYL-N-PHENYL-

**Other names:** Isobutyric acid anilide
Propanamide, 2-methyl-N-phenyl-
i-Butyranilide
**Inchi:** InChI=1S/C10H13NO/c1-8(2)10(12)11-9-6-4-3-5-7-9/h3-8H,1-2H3,(H,11,12)
**InchiKey:** WDRCPKDLZOQCFU-UHFFFAOYSA-N
**Formula:** C10H13NO
**SMILES:** CC(C)C(=O)Nc1ccccc1
**Mol. weight [g/mol]:** 163.22

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -161.94 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 18.87 | kJ/mol | Joback Method |
| hvap | 63.47 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.30 | eV | Cheméo Relay (1.0) |
| log10ws | -1.93 | | Cheméo Relay (1.0) |
| logp | 2.281 | | Crippen Method |
| mcvol | 139.550 | ml/mol | McGowan Method |
| rinpol | 1484.00 | | NIST Webbook |
| rinpol | 1484.00 | | NIST Webbook |
| tb | 522.95 | K | Cheméo Relay (1.0) |
| tf | 332.69 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 324.29 | J/mol×K | 558.48 | Joback Method |
| cpg | 338.54 | J/mol×K | 595.12 | Joback Method |
| cpg | 351.86 | J/mol×K | 631.77 | Joback Method |
| cpg | 364.30 | J/mol×K | 668.41 | Joback Method |
| cpg | 375.89 | J/mol×K | 705.06 | Joback Method |
| cpg | 386.67 | J/mol×K | 741.70 | Joback Method |
| cpg | 396.68 | J/mol×K | 778.35 | Joback Method |

# Sources

| | |
|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C4406411&Units=SI |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |