# Benzeneacetamide, .alpha.-phenyl-

**Inchi:** InChI=1S/C14H13NO/c15-14(16)13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,13H,(H2,15
**InchiKey:** ZXQVXEAZKZFEEP-UHFFFAOYSA-N
**Formula:** C14H13NO
**SMILES:** NC(=O)C(c1ccccc1)c1ccccc1
**Mol. weight [g/mol]:** 211.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -49.65 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 23.37 | kJ/mol | Joback Method |
| hvap | 63.70 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.55 | eV | Cheméo Relay (1.0) |
| log10ws | -3.34 | | Cheméo Relay (1.0) |
| logp | 2.304 | | Crippen Method |
| mcvol | 172.150 | ml/mol | McGowan Method |
| tb | 588.77 | K | Cheméo Relay (1.0) |
| tf | 427.73 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 450.76 | J/mol×K | 699.04 | Joback Method |
| cpg | 465.62 | J/mol×K | 741.95 | Joback Method |
| cpg | 479.13 | J/mol×K | 784.86 | Joback Method |
| cpg | 491.40 | J/mol×K | 827.76 | Joback Method |
| cpg | 502.52 | J/mol×K | 870.67 | Joback Method |
| cpg | 512.59 | J/mol×K | 913.58 | Joback Method |
| cpg | 521.71 | J/mol×K | 956.49 | Joback Method |

## Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C4695130&Units=SI |
| **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):** | |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |