# 2-Butenamide,N-phenyl-

**Inchi:** InChI=1S/C10H11NO/c1-2-6-10(12)11-9-7-4-3-5-8-9/h2-8H,1H3,(H,11,12)/b6-2+
**InchiKey:** BZSYYMAHNJHZCB-QHHAFSJGSA-N
**Formula:** C10H11NO
**SMILES:** CC=CC(=O)Nc1ccccc1
**Mol. weight [g/mol]:** 161.20
**CAS:** 1733-40-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 186.42 | kJ/mol | Joback Method |
| hf | 44.91 | kJ/mol | Joback Method |
| hfus | 22.60 | kJ/mol | Joback Method |
| hvap | 53.27 | kJ/mol | Joback Method |
| ie | 8.70 ± 0.10 | eV | NIST Webbook |
| log10ws | -2.37 | | Crippen Method |
| logp | 2.201 | | Crippen Method |
| mcvol | 135.250 | ml/mol | McGowan Method |
| pc | 3384.14 | kPa | Joback Method |
| tb | 563.08 | K | Joback Method |
| tc | 788.04 | K | Joback Method |
| tf | 326.39 | K | Joback Method |
| vc | 0.508 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 304.56 | J/mol×K | 563.08 | Joback Method |
| cpg | 317.84 | J/mol×K | 600.57 | Joback Method |
| cpg | 330.17 | J/mol×K | 638.07 | Joback Method |
| cpg | 341.62 | J/mol×K | 675.56 | Joback Method |
| cpg | 352.23 | J/mol×K | 713.05 | Joback Method |
| cpg | 362.07 | J/mol×K | 750.54 | Joback Method |
| cpg | 371.19 | J/mol×K | 788.04 | Joback Method |

# Sources

| | |
|---|---|
| **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=C1733400&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

Latest version available from:
https://www.chemeo.com/cid/36-468-3/2-Butenamide-N-phenyl.pdf
Generated by Cheméo on 2024-04-26 15:09:15.123857394 +0000 UTC m=+16433404.044434706.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.