

2-Propenamide, 3-phenyl-

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| Other names: | Cinnamamide 2-Benzylideneacetamide 3-Phenylacrylamide 3-Phenylpropenamide Cinnamide Cinnamic amide Benzylidene acetamide 3-Phenyl-2-propenamide |
| Inchi: | InChI=1S/C9H9NO/c10-9(11)7-6-8-4-2-1-3-5-8/h1-7H,(H2,10,11)/b7-6+ |
| InchiKey: | APEJMQOBVMLION-VOTSOKGWSA-N |
| Formula: | C9H9NO |
| SMILES: | <chem>NC(=O)C=Cc1ccccc1</chem> |
| Mol. weight [g/mol]: | 147.17 |
| CAS: | 621-79-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|---------|----------------|
| chs | -4720.60 | kJ/mol | NIST Webbook |
| gf | 155.06 | kJ/mol | Joback Method |
| hf | 45.87 | kJ/mol | Joback Method |
| hfs | -106.90 | kJ/mol | NIST Webbook |
| hfus | 20.11 | kJ/mol | Joback Method |
| hvap | 55.25 | kJ/mol | Joback Method |
| log10ws | -1.92 | | Crippen Method |
| logp | 1.185 | | Crippen Method |
| mcvol | 121.160 | ml/mol | McGowan Method |
| pc | 4010.84 | kPa | Joback Method |
| tb | 562.56 | K | Joback Method |
| tc | 801.58 | K | Joback Method |
| tf | 345.72 | K | Joback Method |
| vc | 0.447 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 268.31 | J/mol×K | 562.56 | Joback Method |
| cpg | 280.35 | J/mol×K | 602.40 | Joback Method |
| cpg | 291.45 | J/mol×K | 642.23 | Joback Method |
| cpg | 301.67 | J/mol×K | 682.07 | Joback Method |
| cpg | 311.08 | J/mol×K | 721.90 | Joback Method |
| cpg | 319.74 | J/mol×K | 761.74 | Joback Method |
| cpg | 327.72 | J/mol×K | 801.58 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C621794&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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|-----------------|--|
| chs: | Standard solid enthalpy of combustion |
| cpg: | Ideal gas 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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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