

# 4-phenyl-2-buten-1-al

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C10H10O/c11-9-5-4-8-10-6-2-1-3-7-10/h1-7,9H,8H2/b5-4+ |
| <b>InchiKey:</b>            | WLNLUFZWBZXINT-SNAWJCMRSA-N                                    |
| <b>Formula:</b>             | C10H10O  |
| <b>SMILES:</b>              | O=CC=CCc1ccccc1  |
| <b>Mol. weight [g/mol]:</b> | 146.19   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 126.43  | kJ/mol               | Joback Method  |
| hf            | 18.44   | kJ/mol               | Joback Method  |
| hfus          | 18.19   | kJ/mol               | Joback Method  |
| hvap          | 46.81   | kJ/mol               | Joback Method  |
| log10ws       | -2.25   |                      | Crippen Method |
| logp          | 1.984   |                      | Crippen Method |
| mcvol         | 125.270 | ml/mol               | McGowan Method |
| pc            | 3376.28 | kPa                  | Joback Method  |
| ripol         | 1930.00 |                      | NIST Webbook   |
| tb            | 507.70  | K                    | Joback Method  |
| tc            | 727.30  | K                    | Joback Method  |
| tf            | 265.80  | K                    | Joback Method  |
| vc            | 0.484   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 259.95    | J/mol×K | 507.70          | Joback Method |
| cpg           | 316.76    | J/mol×K | 690.70          | Joback Method |
| cpg           | 307.00    | J/mol×K | 654.10          | Joback Method |
| cpg           | 296.48    | J/mol×K | 617.50          | Joback Method |
| cpg           | 285.17    | J/mol×K | 580.90          | Joback Method |
| cpg           | 273.01    | J/mol×K | 544.30          | Joback Method |
| cpg           | 325.84    | J/mol×K | 727.30          | Joback Method |
| dvisc         | 0.0002372 | Paxs    | 507.70          | Joback Method |
| dvisc         | 0.0003037 | Paxs    | 467.38          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0004074 | Paxs | 427.07 | Joback Method |
| dvisc | 0.0005810 | Paxs | 386.75 | Joback Method |
| dvisc | 0.0009000 | Paxs | 346.43 | Joback Method |
| dvisc | 0.0015645 | Paxs | 306.12 | Joback Method |
| dvisc | 0.0032161 | Paxs | 265.80 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R308122&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R308122&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>ripol:</b>   | Polar retention indices                         |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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