

# Allyl cinnamate

|                      |                                                                                                                                                                                                                                                                                          |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 2-Propenoic acid, 3-phenyl-, 2-propenyl ester<br>Cinnamic acid, allyl ester<br>Allyl 3-phenylacrylate<br>Propenyl cinnamate<br>Vinyl carbinyl cinnamate<br>Allylester kyseliny skoricove<br>Allyl 3-phenyl-2-propenoate<br>2-Propenoic acid, 3-phenyl-, 2-propen-1-yl ester<br>NSC 20972 |
| Inchi:               | InChI=1S/C12H12O2/c1-2-10-14-12(13)9-8-11-6-4-3-5-7-11/h2-9H,1,10H2/b9-8+                                                                                                                                                                                                                |
| InchiKey:            | KCMITHMNVLRGJU-CMDGGOBGSA-N                                                                                                                                                                                                                                                              |
| Formula:             | C12H12O2                                                                                                                                                                                                                                                                                 |
| SMILES:              | C=CCOC(=O)C=Cc1ccccc1                                                                                                                                                                                                                                                                    |
| Mol. weight [g/mol]: | 188.22                                                                                                                                                                                                                                                                                   |
| CAS:                 | 1866-31-5                                                                                                                                                                                                                                                                                |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 96.71   | kJ/mol  | Joback Method  |
| hf            | -56.63  | kJ/mol  | Joback Method  |
| hfus          | 22.59   | kJ/mol  | Joback Method  |
| hvap          | 53.03   | kJ/mol  | Joback Method  |
| log10ws       | -2.69   |         | Crippen Method |
| logp          | 2.429   |         | Crippen Method |
| mcvol         | 155.020 | ml/mol  | McGowan Method |
| pc            | 2773.00 | kPa     | Joback Method  |
| rinpol        | 1537.00 |         | NIST Webbook   |
| rinpol        | 1524.00 |         | NIST Webbook   |
| ripol         | 2258.00 |         | NIST Webbook   |
| ripol         | 2258.00 |         | NIST Webbook   |
| tb            | 577.77  | K       | Joback Method  |
| tc            | 797.26  | K       | Joback Method  |
| tf            | 316.74  | K       | Joback Method  |
| vc            | 0.585   | m3/kmol | Joback Method  |

# Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 354.11    | J/mol×K | 577.77          | Joback Method |
| cpg           | 415.30    | J/mol×K | 760.68          | Joback Method |
| cpg           | 404.73    | J/mol×K | 724.10          | Joback Method |
| cpg           | 393.37    | J/mol×K | 687.52          | Joback Method |
| cpg           | 381.18    | J/mol×K | 650.93          | Joback Method |
| cpg           | 368.11    | J/mol×K | 614.35          | Joback Method |
| cpg           | 425.13    | J/mol×K | 797.26          | Joback Method |
| dvisc         | 0.0001620 | Pa×s    | 577.77          | Joback Method |
| dvisc         | 0.0002074 | Pa×s    | 534.26          | Joback Method |
| dvisc         | 0.0002774 | Pa×s    | 490.76          | Joback Method |
| dvisc         | 0.0003927 | Pa×s    | 447.25          | Joback Method |
| dvisc         | 0.0005990 | Pa×s    | 403.75          | Joback Method |
| dvisc         | 0.0010120 | Pa×s    | 360.25          | Joback Method |
| dvisc         | 0.0019746 | Pa×s    | 316.74          | Joback Method |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                       |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1866315&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1866315&amp;Units=SI</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>rinpol:</b> | Non-polar retention indices      |
| <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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