

cis-Allyl cinnamate

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|-----------------------------|---|
| 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-HJWRWDBZSA-N |
| Formula: | C12H12O2 |
| SMILES: | C=CCOC(=O)C=Cc1ccccc1 |
| Mol. weight [g/mol]: | 188.22 |

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 |
| rinsol | 1363.00 | | NIST Webbook |
| tb | 577.77 | K | Joback Method |
| tc | 797.26 | K | Joback Method |
| tf | 316.74 | K | Joback Method |
| vc | 0.585 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 354.11 | J/molxK | 577.77 | Joback Method |
| cpg | 415.30 | J/molxK | 760.68 | Joback Method |
| cpg | 404.73 | J/molxK | 724.10 | Joback Method |
| cpg | 393.37 | J/molxK | 687.52 | Joback Method |
| cpg | 381.18 | J/molxK | 650.93 | Joback Method |
| cpg | 368.11 | J/molxK | 614.35 | Joback Method |
| cpg | 425.13 | J/molxK | 797.26 | Joback Method |
| dvisc | 0.0001620 | Paxs | 577.77 | Joback Method |
| dvisc | 0.0002074 | Paxs | 534.26 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0002774 | Paxs | 490.76 | Joback Method |
| dvisc | 0.0003927 | Paxs | 447.25 | Joback Method |
| dvisc | 0.0005990 | Paxs | 403.75 | Joback Method |
| dvisc | 0.0010120 | Paxs | 360.25 | Joback Method |
| dvisc | 0.0019746 | Paxs | 316.74 | 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=R409557&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| 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 |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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