

3-Methyl-2-buten- 1-yl cinnamate

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|-----------------------------|--|
| Inchi: | InChI=1S/C14H16O2/c1-12(2)10-11-16-14(15)9-8-13-6-4-3-5-7-13/h3-10H,11H2,1-2H3/t |
| InchiKey: | YEGFVCPUCLRIRL-CMDGGGOBGSA-N |
| Formula: | C14H16O2 |
| SMILES: | CC(C)=CCOC(=O)C=Cc1ccccc1 |
| Mol. weight [g/mol]: | 216.28 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 97.38 | kJ/mol | Joback Method |
| hf | -115.91 | kJ/mol | Joback Method |
| hfus | 27.94 | kJ/mol | Joback Method |
| hvap | 58.19 | kJ/mol | Joback Method |
| log10ws | -3.52 | | Crippen Method |
| logp | 3.209 | | Crippen Method |
| mvol | 183.200 | ml/mol | McGowan Method |
| pc | 2320.31 | kPa | Joback Method |
| rinpol | 1792.00 | | NIST Webbook |
| rinpol | 1792.00 | | NIST Webbook |
| tb | 630.89 | K | Joback Method |
| tc | 851.13 | K | Joback Method |
| tf | 322.00 | K | Joback Method |
| vc | 0.697 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 452.00 | J/molxK | 630.89 | Joback Method |
| cpg | 467.53 | J/molxK | 667.60 | Joback Method |
| cpg | 482.04 | J/molxK | 704.30 | Joback Method |
| cpg | 495.58 | J/molxK | 741.01 | Joback Method |
| cpg | 508.22 | J/molxK | 777.72 | Joback Method |
| cpg | 520.02 | J/molxK | 814.43 | Joback Method |
| cpg | 531.05 | J/molxK | 851.13 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R391550&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

Legend

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|------------------|---|
| 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 |
| h vap: | 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 |
| r in pol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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