# (2E)-2-ethyl-3-phenyl-2-propenoic acid

**Inchi:** InChI=1S/C11H12O2/c1-2-10(11(12)13)8-9-6-4-3-5-7-9/h3-8H,2H2,1H3,(H,12,13)/b10-8-

**InchiKey:** RUETZBUVTWCCIZ-CSKARUKUSA-N

**Formula:** C11H12O2

**SMILES:** CCC(=Cc1ccccc1)C(=O)O

**Mol. weight [g/mol]:** 176.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -39.92 | kJ/mol | Joback Method |
| hf | -191.22 | kJ/mol | Joback Method |
| hfus | 22.87 | kJ/mol | Joback Method |
| hvap | 65.82 | kJ/mol | Joback Method |
| log10ws | -2.65 | | Crippen Method |
| logp | 2.565 | | Crippen Method |
| mcvol | 145.230 | ml/mol | McGowan Method |
| pc | 3337.38 | kPa | Joback Method |
| tb | 627.85 | K | Joback Method |
| tc | 836.58 | K | Joback Method |
| tf | 331.86 | K | Joback Method |
| vc | 0.549 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 353.93 | J/mol×K | 627.85 | Joback Method |
| cpg | 365.47 | J/mol×K | 662.64 | Joback Method |
| cpg | 376.24 | J/mol×K | 697.43 | Joback Method |
| cpg | 386.30 | J/mol×K | 732.21 | Joback Method |
| cpg | 395.69 | J/mol×K | 767.00 | Joback Method |
| cpg | 404.47 | J/mol×K | 801.79 | Joback Method |
| cpg | 412.68 | J/mol×K | 836.58 | 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=B6004865&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 |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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