# (E)-4-Phenylbut-3-en-2-yl acetate

**Inchi:** InChI=1S/C12H14O2/c1-10(14-11(2)13)8-9-12-6-4-3-5-7-12/h3-10H,1-2H3/b9-8+
**InchiKey:** DSWDNUYFUXOVBI-CMDGGOBGSA-N
**Formula:** C12H14O2
**SMILES:** CC(=O)OC(C)C=Cc1ccccc1
**Mol. weight [g/mol]:** 190.24

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 6.43 | kJ/mol | Joback Method |
| hf | -187.34 | kJ/mol | Joback Method |
| hfus | 20.34 | kJ/mol | Joback Method |
| hvap | 53.31 | kJ/mol | Joback Method |
| log10ws | -2.94 | | Crippen Method |
| logp | 2.651 | | Crippen Method |
| mcvol | 159.320 | ml/mol | McGowan Method |
| pc | 2676.31 | kPa | Joback Method |
| rinpol | 1460.00 | | NIST Webbook |
| rinpol | 1460.00 | | NIST Webbook |
| tb | 580.65 | K | Joback Method |
| tc | 800.23 | K | Joback Method |
| tf | 303.50 | K | Joback Method |
| vc | 0.598 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 374.76 | J/mol×K | 580.65 | Joback Method |
| cpg | 389.79 | J/mol×K | 617.25 | Joback Method |
| cpg | 403.87 | J/mol×K | 653.84 | Joback Method |
| cpg | 417.03 | J/mol×K | 690.44 | Joback Method |
| cpg | 429.31 | J/mol×K | 727.04 | Joback Method |
| cpg | 440.76 | J/mol×K | 763.63 | Joback Method |
| cpg | 451.41 | J/mol×K | 800.23 | Joback Method |
| dvisc | 0.0027204 | Pa×s | 303.50 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0012128 | Pa×s | 349.69 | Joback Method |
| dvisc | 0.0006529 | Pa×s | 395.88 | Joback Method |
| dvisc | 0.0004000 | Pa×s | 442.07 | Joback Method |
| dvisc | 0.0002689 | Pa×s | 488.27 | Joback Method |
| dvisc | 0.0001936 | Pa×s | 534.46 | Joback Method |
| dvisc | 0.0001469 | Pa×s | 580.65 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R341307&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |