# Benzenemethanol, «alpha»-methyl-, propanoate

**Other names:** 1-Phenylethyl propionate
Benzyl alcohol, «alpha»-methyl-, propionate
Benzyl alcohol, Â«alphaÂ»-methyl-, propionate
Methylphenylcarbinyl propionate
NSC 406571
Phenylmethylcarbinyl propionate
Propionic acid, «alpha»-methylbenzyl ester
Propionic acid, Â«alphaÂ»-methylbenzyl ester
Styrallyl propionate
«alpha»-Methylbenzyl alcohol, propionate
«alpha»-Methylbenzyl propanoate
«alpha»-Methylbenzyl propionate
Â«alphaÂ»-Methylbenzyl alcohol, propionate
Â«alphaÂ»-Methylbenzyl propanoate
Â«alphaÂ»-Methylbenzyl propionate

**Inchi:** InChI=1S/C11H14O2/c1-3-11(12)13-9(2)10-7-5-4-6-8-10/h4-9H,3H2,1-2H3

**InchiKey:** WCIQNYOXLZQQMU-UHFFFAOYSA-N

**Formula:** C11H14O2

**SMILES:** CCC(=O)OC(C)c1ccccc1

**Mol. weight [g/mol]:** 178.23

**CAS:** 120-45-6

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -82.21 | kJ/mol | Joback Method |
| hf | -283.92 | kJ/mol | Joback Method |
| hfus | 17.55 | kJ/mol | Joback Method |
| hvap | 51.12 | kJ/mol | Joback Method |
| log10ws | -2.85 | | Crippen Method |
| logp | 2.701 | | Crippen Method |
| mcvol | 149.530 | ml/mol | McGowan Method |
| pc | 2802.44 | kPa | Joback Method |
| tb | 553.61 | K | Joback Method |
| tc | 767.42 | K | Joback Method |
| tf | 297.31 | K | Joback Method |
| vc | 0.561 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 423.32 | J/mol×K | 767.42 | Joback Method |
| cpg | 346.73 | J/mol×K | 553.61 | Joback Method |
| cpg | 361.56 | J/mol×K | 589.25 | Joback Method |
| cpg | 375.53 | J/mol×K | 624.88 | Joback Method |
| cpg | 388.67 | J/mol×K | 660.52 | Joback Method |
| cpg | 401.00 | J/mol×K | 696.15 | Joback Method |
| cpg | 412.55 | J/mol×K | 731.79 | Joback Method |
| dvisc | 0.0001883 | Pa×s | 553.61 | Joback Method |
| dvisc | 0.0030377 | Pa×s | 297.31 | Joback Method |
| dvisc | 0.0014284 | Pa×s | 340.03 | Joback Method |
| dvisc | 0.0007949 | Pa×s | 382.74 | Joback Method |
| dvisc | 0.0004976 | Pa×s | 425.46 | Joback Method |
| dvisc | 0.0003393 | Pa×s | 468.18 | Joback Method |
| dvisc | 0.0002466 | Pa×s | 510.89 | Joback Method |
| rfi | 1.48650 | | 298.20 | Ternary liquid liquid equilibria for mixtures of an ionic liquid + n-hexane + an organic compound involved in the kinetic resolution of rac-1-phenyl ethanol (rac-1-phenyl ethanol, vinyl propionate, rac-1-phenylethyl propionate or propionic acid) at 298.2K and atmospheric pressure |

# Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Ternary liquid liquid equilibria for mixtures of an ionic liquid + n-hexane + an organic compound involved in the kinetic resolution of rac-1-phenyl ethanol (rac-1-phenyl ethanol, vinyl propionate, rac-1-phenylethyl propionate or propionic acid) at 298.2K and atmospheric pressure:** https://www.doi.org/10.1016/j.fluid.2007.10.011

**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=C120456&Units=SI

# 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 |
| **rfi:** | Refractive Index |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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