# Benzoic acid, 2-methylpropyl ester

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|---|---|
| **Other names:** | Benzoic acid, isobutyl ester |
| | Isobutyl benzoate |
| | 2-methylpropyl benzoate |
| **Inchi:** | InChI=1S/C11H14O2/c1-9(2)8-13-11(12)10-6-4-3-5-7-10/h3-7,9H,8H2,1-2H3 |
| **InchiKey:** | KYZHGEFMXZOSJN-UHFFFAOYSA-N |
| **Formula:** | C11H14O2 |
| **SMILES:** | CC(C)COC(=O)c1ccccc1 |
| **Mol. weight [g/mol]:** | 178.23 |
| **CAS:** | 120-50-3 |

# 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 | -2.73 | | Crippen Method |
| logp | 2.499 | | Crippen Method |
| mcvol | 149.530 | ml/mol | McGowan Method |
| pc | 2802.44 | kPa | Joback Method |
| rinpol | 1331.20 | | NIST Webbook |
| rinpol | 1308.00 | | NIST Webbook |
| rinpol | 1319.00 | | NIST Webbook |
| rinpol | 1312.00 | | NIST Webbook |
| rinpol | 1318.00 | | NIST Webbook |
| rinpol | 1327.00 | | NIST Webbook |
| rinpol | 1315.00 | | NIST Webbook |
| rinpol | 1305.00 | | NIST Webbook |
| rinpol | 1310.00 | | NIST Webbook |
| rinpol | 1312.00 | | NIST Webbook |
| rinpol | 1318.00 | | NIST Webbook |
| rinpol | 1331.20 | | NIST Webbook |
| rinpol | 1308.00 | | NIST Webbook |
| rinpol | 1298.00 | | NIST Webbook |
| rinpol | 1308.00 | | NIST Webbook |
| rinpol | 1326.00 | | NIST Webbook |
| rinpol | 1306.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 1306.00 | | NIST Webbook |
| rinpol | 1302.00 | | NIST Webbook |
| rinpol | 1331.00 | | NIST Webbook |
| rinpol | 1311.00 | | NIST Webbook |
| rinpol | 1315.00 | | NIST Webbook |
| rinpol | 1310.00 | | NIST Webbook |
| ripol | 1817.00 | | NIST Webbook |
| ripol | 1808.00 | | NIST Webbook |
| ripol | 1771.00 | | NIST Webbook |
| ripol | 1815.00 | | NIST Webbook |
| ripol | 1789.00 | | NIST Webbook |
| ripol | 1800.00 | | NIST Webbook |
| ripol | 1785.00 | | NIST Webbook |
| ripol | 1806.00 | | NIST Webbook |
| ripol | 1801.00 | | NIST Webbook |
| ripol | 1811.00 | | NIST Webbook |
| ripol | 1830.00 | | NIST Webbook |
| ripol | 1776.00 | | NIST Webbook |
| ripol | 1799.00 | | NIST Webbook |
| tb | 510.15 ± 1.50 | K | NIST Webbook |
| tb | 514.65 ± 1.00 | K | NIST Webbook |
| tb | 515.30 ± 0.30 | K | NIST Webbook |
| tb | 515.20 | K | NIST Webbook |
| tb | 515.30 ± 0.50 | K | NIST Webbook |
| tb | 515.29 ± 0.40 | K | NIST Webbook |
| tb | 515.05 ± 0.50 | K | NIST Webbook |
| 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 | 401.00 | J/mol×K | 696.15 | Joback Method |
| cpg | 423.32 | J/mol×K | 767.42 | Joback Method |
| cpg | 412.55 | J/mol×K | 731.79 | 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 |
| dvisc | 0.0001883 | Pa×s | 553.61 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003393 | Pa×s | 468.18 | Joback Method |
| dvisc | 0.0002466 | Pa×s | 510.89 | 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 |
| hvapt | 59.10 | kJ/mol | 374.00 | NIST Webbook |
| hvapt | 55.70 | kJ/mol | 424.00 | NIST Webbook |
| hvapt | 63.20 | kJ/mol | 424.00 | NIST Webbook |

# 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=C120503&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
**hvapt:** Enthalpy of vaporization at a given temperature
**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
**ripol:** Polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume