

Benzoic acid, 2-methyl-

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|-----------------------------|--|
| Other names: | 2-Methylbenzoic acid Orthotoluic acid o-Methylbenzoic acid o-Toluic acid o-Toluylic acid |
| Inchi: | InChI=1S/C8H8O2/c1-6-4-2-3-5-7(6)8(9)10/h2-5H,1H3,(H,9,10) |
| InchiKey: | ZWLPBLYKEWSWPD-UHFFFAOYSA-N |
| Formula: | C8H8O2 |
| SMILES: | Cc1ccccc1C(=O)O |
| Mol. weight [g/mol]: | 136.15 |
| CAS: | 118-90-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-----------------|--------|--------------------------------------|
| affp | 838.80 | kJ/mol | NIST Webbook |
| basg | 807.80 | kJ/mol | NIST Webbook |
| chs | -3864.00 | kJ/mol | NIST Webbook |
| chs | -3874.90 ± 0.80 | kJ/mol | NIST Webbook |
| chs | -3874.40 ± 4.60 | kJ/mol | NIST Webbook |
| chs | -3875.00 ± 0.75 | kJ/mol | NIST Webbook |
| chs | -3858.00 | kJ/mol | NIST Webbook |
| gf | -146.48 | kJ/mol | Joback Method |
| hf | -320.60 | kJ/mol | NIST Webbook |
| hf | -320.60 ± 1.50 | kJ/mol | NIST Webbook |
| hf | -331.20 | kJ/mol | NIST Webbook |
| hfs | -416.50 ± 0.92 | kJ/mol | NIST Webbook |
| hfs | -416.50 ± 1.50 | kJ/mol | NIST Webbook |
| hfs | -427.10 ± 3.80 | kJ/mol | NIST Webbook |
| hfus | 15.81 | kJ/mol | Joback Method |
| hsub | 95.90 ± 0.10 | kJ/mol | NIST Webbook |
| hsub | 95.90 | kJ/mol | NIST Webbook |
| hsub | 95.90 ± 0.10 | kJ/mol | NIST Webbook |
| hvap | 59.77 | kJ/mol | Joback Method |
| ie | 9.10 | eV | NIST Webbook |
| ie | 9.40 | eV | NIST Webbook |
| log10ws | -2.06 | | Aqueous Solubility Prediction Method |

| | | | |
|-------|---------------|---------|---|
| logp | 1.693 | | Crippen Method |
| mcvol | 107.260 | ml/mol | McGowan Method |
| pc | 4356.87 | kPa | Joback Method |
| tb | 531.70 | K | NIST Webbook |
| tc | 763.00 | K | Vapor-liquid critical point measurements of fifteen compounds by the pulse-heating method |
| tf | 376.50 ± 0.05 | K | NIST Webbook |
| tf | 377.65 ± 2.00 | K | NIST Webbook |
| tf | 376.90 ± 0.30 | K | NIST Webbook |
| tf | 377.63 | K | Aqueous Solubility Prediction Method |
| tf | 380.00 ± 1.50 | K | NIST Webbook |
| vc | 0.401 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 283.75 | J/mol×K | 767.50 | Joback Method |
| cpg | 277.03 | J/mol×K | 732.94 | Joback Method |
| cpg | 269.83 | J/mol×K | 698.38 | Joback Method |
| cpg | 262.13 | J/mol×K | 663.82 | Joback Method |
| cpg | 253.91 | J/mol×K | 629.27 | Joback Method |
| cpg | 245.16 | J/mol×K | 594.71 | Joback Method |
| cpg | 235.84 | J/mol×K | 560.15 | Joback Method |
| cps | 174.90 | J/mol×K | 298.00 | NIST Webbook |
| dvisc | 0.0002839 | Paxs | 483.30 | Joback Method |
| dvisc | 0.0001794 | Paxs | 521.73 | Joback Method |
| dvisc | 0.0001208 | Paxs | 560.15 | Joback Method |
| dvisc | 0.0019990 | Paxs | 368.03 | Joback Method |
| dvisc | 0.0009222 | Paxs | 406.46 | Joback Method |
| dvisc | 0.0004863 | Paxs | 444.88 | Joback Method |
| dvisc | 0.0051891 | Paxs | 329.61 | Joback Method |
| hfust | 20.17 | kJ/mol | 376.90 | NIST Webbook |
| hfust | 20.17 | kJ/mol | 376.90 | NIST Webbook |
| hfust | 20.17 | kJ/mol | 376.90 | NIST Webbook |

| | | | | |
|------|------|-----|--------|--|
| psub | 0.05 | kPa | 361.20 | Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods |
| psub | 0.04 | kPa | 358.70 | Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods |
| psub | 0.04 | kPa | 358.60 | Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods |
| psub | 0.07 | kPa | 364.20 | Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods |
| psub | 0.08 | kPa | 367.40 | Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods |
| psub | 0.13 | kPa | 373.00 | Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods |
| psub | 0.03 | kPa | 355.40 | Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods |

| | | | | |
|-------|----------|---------|--------|--|
| psub | 0.02 | kPa | 348.20 | Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods |
| psub | 0.01 | kPa | 345.20 | Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods |
| psub | 7.67e-03 | kPa | 341.20 | Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods |
| psub | 4.21e-03 | kPa | 335.20 | Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods |
| psub | 2.80e-03 | kPa | 331.20 | Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods |
| psub | 0.02 | kPa | 351.20 | Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods |
| sfust | 53.50 | J/mol×K | 376.90 | NIST Webbook |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.54533e+01 |
| Coeff. B | -4.69014e+03 |
| Coeff. C | -9.91310e+01 |
| Temperature range (K), min. | 376.85 |
| Temperature range (K), max. | 561.58 |

| Information | Value |
|-----------------------------|--|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$ |
| Coeff. A | 1.31614e+02 |
| Coeff. B | -1.40488e+04 |
| Coeff. C | -1.62792e+01 |
| Coeff. D | 5.55990e-06 |
| Temperature range (K), min. | 376.85 |
| Temperature range (K), max. | 751.00 |

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Solubilities of Phthalic Acid and o-Toluic Acid in Binary Acetic Acid + Water Method
Solvent Mixtures:
RDB:

<https://www.doi.org/10.1021/acs.jced.6b00324>

https://en.wikipedia.org/wiki/Joback_method

<https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=956>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C118901&Units=SI>

Vapor-liquid critical point measurements of fifteen compounds
The Yaws Handbook of Vapor Pressure:

<https://www.doi.org/10.1016/j.fluid.2014.07.038>

KDB Vapor Pressure Data:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Pressure:
KDB Vapor Pressure Data:

<https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=956>

Solubilities of Benzoic Acid, p-Methylbenzoic Acid,

<https://www.doi.org/10.1021/je700677d>

Benzoyl Acid Derivatives: Evaluation of thermophysical properties with aqueous solubility prediction Method:
McGowan Method:

<https://www.doi.org/10.1016/j.tca.2015.03.026>

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

<http://link.springer.com/article/10.1007/BF02311772>

Legend

affp:

Proton affinity

| | |
|-----------------|--|
| basg: | Gas basicity |
| chs: | Standard solid enthalpy of combustion |
| cpg: | Ideal gas heat capacity |
| cps: | Solid phase heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfs: | Solid phase enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hfust: | Enthalpy of fusion at a given temperature |
| hsub: | Enthalpy of sublimation at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| ie: | Ionization energy |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| psub: | Sublimation pressure |
| pvap: | Vapor pressure |
| sfust: | Entropy of fusion at a given temperature |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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