

Isophthalic acid

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| Other names: | 1,3-Benzenedicarboxylic acid Acide isophthalique Benzene,1,3-dicarboxylic acid IPA Kyselina isoftalova NSC 15310 m-Benzenedicarboxylic acid m-Dicarboxybenzene m-Phthalic acid |
| Inchi: | InChI=1S/C8H6O4/c9-7(10)5-2-1-3-6(4-5)8(11)12/h1-4H,(H,9,10)(H,11,12) |
| InchiKey: | QQVIHTHCMHWDBS-UHFFFAOYSA-N |
| Formula: | C8H6O4 |
| SMILES: | O=C(O)c1ccccc(C(=O)O)c1 |
| Mol. weight [g/mol]: | 166.13 |
| CAS: | 121-91-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-----------------|--------|----------------|
| chs | -3215.37 | kJ/mol | NIST Webbook |
| chs | -3202.60 ± 0.50 | kJ/mol | NIST Webbook |
| chs | -3217.85 | kJ/mol | NIST Webbook |
| chs | -3204.10 ± 1.50 | kJ/mol | NIST Webbook |
| gf | -412.22 | kJ/mol | Joback Method |
| hf | -513.01 | kJ/mol | Joback Method |
| hfs | -801.50 ± 1.50 | kJ/mol | NIST Webbook |
| hfs | -803.04 | kJ/mol | NIST Webbook |
| hfus | 21.50 | kJ/mol | Joback Method |
| hsub | 142.00 ± 0.70 | kJ/mol | NIST Webbook |
| hvap | 83.19 | kJ/mol | Joback Method |
| ie | 10.00 ± 0.20 | eV | NIST Webbook |
| log10ws | -1.59 | | Crippen Method |
| logp | 1.083 | | Crippen Method |
| mcvol | 114.700 | ml/mol | McGowan Method |
| pc | 5406.57 | kPa | Joback Method |
| tb | 706.20 | K | Joback Method |
| tc | 907.67 | K | Joback Method |

| | | | |
|----|--------|---------|---|
| tf | 621.20 | K | Solid-Liquid Equilibria for Benzoic Acid + p-Toluic Acid + Chloroform, Benzoic Acid + p-Toluic Acid + Acetic Acid, and Terephthalic Acid + Isophthalic Acid + N,N-Dimethylformamide |
| vc | 0.425 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------------|---------|-----------------|---------------|
| cpg | 311.15 | J/mol×K | 874.09 | Joback Method |
| cpg | 301.12 | J/mol×K | 806.93 | Joback Method |
| cpg | 306.34 | J/mol×K | 840.51 | Joback Method |
| cpg | 315.57 | J/mol×K | 907.67 | Joback Method |
| cpg | 282.80 | J/mol×K | 706.20 | Joback Method |
| cpg | 289.37 | J/mol×K | 739.78 | Joback Method |
| cpg | 295.47 | J/mol×K | 773.36 | Joback Method |
| cps | 201.70 | J/mol×K | 323.00 | NIST Webbook |
| cps | 201.70 | J/mol×K | 323.00 | NIST Webbook |
| dvisc | 0.0000196 | Paxs | 706.20 | Joback Method |
| dvisc | 0.0001006 | Paxs | 573.28 | Joback Method |
| dvisc | 0.0000539 | Paxs | 617.59 | Joback Method |
| dvisc | 0.0000314 | Paxs | 661.89 | Joback Method |
| dvisc | 0.0013822 | Paxs | 440.36 | Joback Method |
| dvisc | 0.0004918 | Paxs | 484.67 | Joback Method |
| dvisc | 0.0002081 | Paxs | 528.97 | Joback Method |
| hfust | 43.20 | kJ/mol | 617.40 | NIST Webbook |
| hsubt | 106.70 ± 2.20 | kJ/mol | 528.00 | NIST Webbook |
| hsubt | 114.20 | kJ/mol | 528.00 | NIST Webbook |
| hsubt | 134.60 ± 1.60 | kJ/mol | 450.00 | NIST Webbook |

Correlations

| Information | Value |
|---------------|--|
| Property code | pvap |
| Equation | $\ln(P_{\text{vap}}) = A + B/T + C*\ln(T) + D*T^2$ |
| Coeff. A | 2.32607e+02 |

| | |
|-----------------------------|--------------|
| Coeff. B | -2.87138e+04 |
| Coeff. C | -2.91467e+01 |
| Coeff. D | 5.64805e-06 |
| Temperature range (K), min. | 619.15 |
| Temperature range (K), max. | 1007.00 |

Sources

Solubilities of Terephthalic Acid, Phthalic Acid, and Isophthalic Acid in Ternary Mixtures; Cyclohexanone, 1,2-Diethoxyethane, and Acetophenone; McGowan Method:

<https://www.doi.org/10.1021/je9001976>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C121915&Units=SI>

NIST Webbook:

Measurements of the solubilities of m-phthalic acid in acetone, ethanol and understanding the enhanced solubility of 1,3-benzenedicarboxylic acid in Solubilities of 1,2-benzenedicarboxylic acid in Water at Various Temperature: Joback Method:

<https://www.doi.org/10.1016/j.fluid.2008.01.014>

<https://www.doi.org/10.1016/j.jct.2016.10.011>

<https://www.doi.org/10.1021/je049784c>

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

Measurement and Correlation of the Solubilities of m-Phthalic Acid in Molar Vapor Pressure Data:

<https://www.doi.org/10.1021/je800520w>

<https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=968>

Solubilities of Isophthalic Acid in Ternary Mixtures of Acetic Acid + Water Please provide wpa192.53.16.219:8080 for the System of Benzene Dicarboxylic Acid + Methanol and prediction of solid-liquid phase equilibrium for Grunewald Method:

<https://www.doi.org/10.1021/acs.jced.7b00958>

<https://www.doi.org/10.1021/je500542j>

<https://www.doi.org/10.1016/j.fluid.2015.03.042>

https://www.chemeo.com/doc/models/crippen_log10ws

<https://www.doi.org/10.1021/je049801y>

<https://www.doi.org/10.1021/je101319f>

<https://www.doi.org/10.1021/je800353s>

1,3,5-Benzenetricarboxylic Acid and 1,3-Benzenedicarboxylic Acid in Acetic Acid + Water Solvent Mixtures:

Legend

| | |
|---------------|--|
| 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 |

| | |
|-----------------|---|
| hsubt: | Enthalpy of sublimation at a given temperature |
| 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 |
| pvap: | Vapor pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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