# 2-Propenoic acid, 2-methyl-

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|---|---|
| **Other names:** | .alpha.-methylacrylic acid |
| | 2-Methyl-2-propenoic acid |
| | 2-Methylacrylic acid |
| | 2-Methylpropenoic acid |
| | ALPHA-METHYLACRYLIC ACID |
| | Acrylic acid, 2-methyl- |
| | CH2=C(CH3)COOH |
| | Kyselina methakrylova |
| | Methacrylic acid |
| | Methacrylic acid glacial |
| | Methylacrylic acid |
| | NSC 7393 |
| | Propionic acid, 2-methylene- |
| | «alpha»-Methacrylic acid |
| | «alpha»-Methylacrylic acid |
| | Â«alphaÂ»-Methacrylic acid |
| | Â«alphaÂ»-Methylacrylic acid |
| **Inchi:** | InChI=1S/C4H6O2/c1-3(2)4(5)6/h1H2,2H3,(H,5,6) |
| **InchiKey:** | CERQOIWHTDAKMF-UHFFFAOYSA-N |
| **Formula:** | C4H6O2 |
| **SMILES:** | C=C(C)C(=O)O |
| **Mol. weight [g/mol]:** | 86.09 |
| **CAS:** | 79-41-4 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 816.70 | kJ/mol | NIST Webbook |
| basg | 785.70 | kJ/mol | NIST Webbook |
| chl | -2012.00 ± 0.40 | kJ/mol | NIST Webbook |
| chl | -2016.70 ± 2.20 | kJ/mol | NIST Webbook |
| gf | -203.65 | kJ/mol | Joback Method |
| hf | -372.20 | kJ/mol | NIST Webbook |
| hf | -367.30 ± 2.40 | kJ/mol | NIST Webbook |
| hfl | -419.70 ± 0.40 | kJ/mol | NIST Webbook |
| hfl | -414.80 ± 2.30 | kJ/mol | NIST Webbook |
| hfus | 9.21 | kJ/mol | Joback Method |
| hvap | 47.50 ± 0.40 | kJ/mol | NIST Webbook |

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|---|---|---|---|
| hvap | 47.50 ± 0.40 | kJ/mol | NIST Webbook |
| hvap | 47.50 | kJ/mol | NIST Webbook |
| ie | 10.15 | eV | NIST Webbook |
| log10ws | 0.01 | | Aqueous Solubility Prediction Method |
| logp | 0.647 | | Crippen Method |
| mcvol | 70.360 | ml/mol | McGowan Method |
| nfpaf | %!d(float64=2) | | KDB |
| nfpah | %!d(float64=3) | | KDB |
| nfpas | %!d(float64=2) | | KDB |
| pc | 4905.21 ± 100.00 | kPa | NIST Webbook |
| rinpol | 711.00 | | NIST Webbook |
| tb | 435.70 | K | NIST Webbook |
| tc | 638.40 ± 3.00 | K | NIST Webbook |
| tf | 229.87 | K | Joback Method |
| vc | 0.267 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 130.74 | J/mol×K | 433.53 | Joback Method |
| cpg | 136.67 | J/mol×K | 463.66 | Joback Method |
| cpg | 142.32 | J/mol×K | 493.79 | Joback Method |
| cpg | 147.70 | J/mol×K | 523.92 | Joback Method |
| cpg | 152.83 | J/mol×K | 554.05 | Joback Method |
| cpg | 157.71 | J/mol×K | 584.18 | Joback Method |
| cpg | 162.35 | J/mol×K | 614.31 | Joback Method |
| cpl | 159.70 | J/mol×K | 298.15 | NIST Webbook |
| cpl | 159.70 | J/mol×K | 298.15 | NIST Webbook |
| dvisc | 0.0009450 | Pa×s | 318.15 | Densities and Viscosities for Binary Mixtures of Ethyl Lactate with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate at (298.15, 308.15, and 318.15) K |

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|---|---|---|---|---|
| dvisc | 0.0010780 | Pa×s | 308.15 | Densities and Viscosities of Binary Mixtures of Propylene Glycol Monomethyl Ether Acetate with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate between 298.15 K and 318.15 K |
| dvisc | 0.0009450 | Pa×s | 318.15 | Densities and Viscosities of Binary Mixtures of Propylene Glycol Monomethyl Ether Acetate with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate between 298.15 K and 318.15 K |
| dvisc | 0.0012670 | Pa×s | 298.15 | Density and Viscosity for Ethyl 3-Ethoxypropionate + Methacrylic Acid, + Benzyl Methacrylate, and + 2-Hydroxyethyl Methacrylate |
| dvisc | 0.0010780 | Pa×s | 308.15 | Density and Viscosity for Ethyl 3-Ethoxypropionate + Methacrylic Acid, + Benzyl Methacrylate, and + 2-Hydroxyethyl Methacrylate |
| dvisc | 0.0009450 | Pa×s | 318.15 | Density and Viscosity for Ethyl 3-Ethoxypropionate + Methacrylic Acid, + Benzyl Methacrylate, and + 2-Hydroxyethyl Methacrylate |

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|---|---|---|---|---|
| dvisc | 0.0012670 | Pa×s | 298.15 | Excess Molar Volumes and Viscosities for Binary Mixtures of Cyclohexanone with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate at (298.15, 308.15, and 318.15) K |
| dvisc | 0.0010780 | Pa×s | 308.15 | Excess Molar Volumes and Viscosities for Binary Mixtures of Cyclohexanone with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate at (298.15, 308.15, and 318.15) K |
| dvisc | 0.0009450 | Pa×s | 318.15 | Excess Molar Volumes and Viscosities for Binary Mixtures of Cyclohexanone with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate at (298.15, 308.15, and 318.15) K |
| dvisc | 0.0012670 | Pa×s | 298.15 | Densities and Viscosities of Binary Mixtures of Propylene Glycol Monomethyl Ether Acetate with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate between 298.15 K and 318.15 K |

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|---|---|---|---|---|---|
| dvisc | 0.0012670 | Pa×s | 298.15 | Densities and Viscosities of Binary Mixtures of 1-Butanol with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate between 288.15 K and 318.15 K | |
| dvisc | 0.0010780 | Pa×s | 308.15 | Densities and Viscosities of Binary Mixtures of 1-Butanol with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate between 288.15 K and 318.15 K | |
| dvisc | 0.0009450 | Pa×s | 318.15 | Densities and Viscosities of Binary Mixtures of 1-Butanol with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate between 288.15 K and 318.15 K | |
| dvisc | 0.0012670 | Pa×s | 298.15 | Excess Molar Volumes and Viscosities for Binary Mixtures of Propylene Glycol Monomethyl Ether with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate at (298.15, 308.15, and 318.15) K | |

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|---|---|---|---|---|---|
| dvisc | 0.0010780 | Pa×s | 308.15 | Excess Molar Volumes and Viscosities for Binary Mixtures of Propylene Glycol Monomethyl Ether with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate at (298.15, 308.15, and 318.15) K | |
| dvisc | 0.0009450 | Pa×s | 318.15 | Excess Molar Volumes and Viscosities for Binary Mixtures of Propylene Glycol Monomethyl Ether with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate at (298.15, 308.15, and 318.15) K | |
| dvisc | 0.0012670 | Pa×s | 298.15 | Densities and Viscosities for Binary Mixtures of Ethyl Lactate with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate at (298.15, 308.15, and 318.15) K | |
| dvisc | 0.0010780 | Pa×s | 308.15 | Densities and Viscosities for Binary Mixtures of Ethyl Lactate with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate at (298.15, 308.15, and 318.15) K | |

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|---|---|---|---|---|---|
| dvisc | 0.0014470 | Pa×s | 288.15 | Densities and Viscosities of Binary Mixtures of 1-Butanol with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate between 288.15 K and 318.15 K | |
| hfust | 8.06 | kJ/mol | 287.50 | NIST Webbook | |
| hfust | 8.06 | kJ/mol | 287.50 | NIST Webbook | |
| hvapt | 53.90 | kJ/mol | 378.00 | NIST Webbook | |
| hvapt | 51.60 | kJ/mol | 366.00 | NIST Webbook | |
| rhol | 1009.13 | kg/m3 | 298.15 | Densities and derived thermodynamic properties of the binary systems of 1,1-dimethylethyl methyl ether with allyl methacrylate, butyl methacrylate, methacrylic acid, and vinyl acetate at T = (298.15 and 308.15) K | |
| rhol | 998.64 | kg/m3 | 308.15 | Densities and derived thermodynamic properties of the binary systems of 1,1-dimethylethyl methyl ether with allyl methacrylate, butyl methacrylate, methacrylic acid, and vinyl acetate at T = (298.15 and 308.15) K | |
| rhol | 1009.13 | kg/m3 | 298.15 | Densities, isobaric thermal compressibilities and derived thermodynamic properties of the binary systems of cyclohexane with allyl methacrylate, butyl methacrylate, methacrylic acid, and vinyl acetate at t = (298.15 and 308.15)K | |

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|---|---|---|---|---|
| rhol | 998.64 | kg/m3 | 308.15 | Densities, isobaric thermal compressibilities and derived thermodynamic properties of the binary systems of cyclohexane with allyl methacrylate, butyl methacrylate, methacrylic acid, and vinyl acetate at t = (298.15 and 308.15)K |
| sfust | 28.04 | J/mol×K | 287.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.46680e+01 |
| Coeff. B | -3.49650e+03 |
| Coeff. C | -8.77770e+01 |
| Temperature range (K), min. | 330.92 |
| Temperature range (K), max. | 461.47 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 2.54171e+01 |
| Coeff. B | -6.95597e+03 |
| Coeff. C | -6.39603e-01 |
| Coeff. D | -4.86105e-06 |
| Temperature range (K), min. | 288.15 |
| Temperature range (K), max. | 643.00 |

# Sources

**Excess Molar Volumes and Viscosities for Binary Mixtures of Cyclohexanone with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate at (298.15, 308.15, and 318.15) K:** https://www.doi.org/10.1021/je0502389

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|---|---|
| Densities and Viscosities of Binary Mixtures of 1-Butanol with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate between 288.15 K and 318.15 K: | https://www.doi.org/10.1021/je0601255 |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| Excess Molar Volumes and Viscosities for Binary Mixtures of Propylene Glycol Monomethyl Ether with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate at (298.15, 308.15, and 318.15) K: | https://www.doi.org/10.1021/je060288t |
| KDB Vapor Pressure Data: | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=976 |
| Densities and derived thermodynamic properties of the binary systems of cyclohexane with allyl methacrylate, butyl methacrylate, and 2-ethoxyethyl methacrylate at T = (298.15 and 308.15) K: | https://www.doi.org/10.1016/j.jct.2004.11.012 |
| Liquid-liquid equilibrium data for the binary system methacrylic acid + 1,1-dimethylethyl methylether with allyl methacrylate, butyl methacrylate, and 2-ethoxyethyl methacrylate at T = (298.15 and 308.15) K: | https://www.doi.org/10.1016/j.fluid.2011.09.002 |
| Aqueous Solubility Prediction Methodology based on Physicochemical Properties of Ionized and Non-ionized Species at 298 K: | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| Densities, isobaric thermal compressibilities and derived thermodynamic properties of the binary systems of cyclohexane with allyl methacrylate, butyl methacrylate, and 2-ethoxyethyl methacrylate at T = (298.15 and 308.15) K: | https://www.doi.org/10.1016/j.tca.2005.06.007 |
| Density and Viscosity for Ethyl 3-Ethoxypropionate + Methacrylic Acid, Benzyl Methacrylate, Butyl Methacrylate, and 2-Ethoxyethyl Methacrylate at t = (298.15 and 308.15)K: | https://www.doi.org/10.1021/je050223a |
| The Yaws Handbook of Vapor Pressure: | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| Phase Equilibrium Measurements of the Methacrolein-Methacrylic Acid-Water Ternary System at 101.3 kPa: | https://www.doi.org/10.1021/acs.jced.9b00649 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C79414&Units=SI |
| KDB: | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=976 |
| Densities and Viscosities of Binary Mixtures of Propylene Glycol Monomethyl Ether Acetate with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate at (298.15, 308.15, and 318.15) K: | https://www.doi.org/10.1021/je050196o |
| Densities and Viscosities for Binary Mixtures of Ethyl Lactate with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate at (298.15, 308.15, and 318.15) K: | https://www.doi.org/10.1021/je600568w |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| Crippen method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **nfpaf:** | NFPA Fire Rating |
| **nfpah:** | NFPA Health Rating |
| **nfpas:** | NFPA Safety Rating |
| **pc:** | Critical Pressure |

| | |
|---|---|
| **pvap:** | Vapor pressure |
| **rhol:** | Liquid Density |
| **rinpol:** | Non-polar retention indices |
| **sfust:** | Entropy of fusion at a given temperature |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |