# Propanamide, 2-methyl-

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|---|---|
| **Other names:** | 2-methylpropanamide |
| | 2-methylpropionamide |
| | C-isopropylformamide |
| | isobutyramide |
| **Inchi:** | InChI=1S/C4H9NO/c1-3(2)4(5)6/h3H,1-2H3,(H2,5,6) |
| **InchiKey:** | WFKAJVHLWXSISD-UHFFFAOYSA-N |
| **Formula:** | C4H9NO |
| **SMILES:** | CC(C)C(N)=O |
| **Mol. weight [g/mol]:** | 87.12 |
| **CAS:** | 563-83-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 878.60 | kJ/mol | NIST Webbook |
| basg | 850.00 ± 6.00 | kJ/mol | NIST Webbook |
| basg | 851.00 ± 3.00 | kJ/mol | NIST Webbook |
| basg | 846.70 | kJ/mol | NIST Webbook |
| chs | -2491.70 ± 0.60 | kJ/mol | NIST Webbook |
| gf | -82.11 | kJ/mol | Joback Method |
| hf | -282.60 ± 0.90 | kJ/mol | NIST Webbook |
| hfs | -368.60 ± 0.90 | kJ/mol | NIST Webbook |
| hfus | 19.20 | kJ/mol | Heat Capacities and Enthalpies of Solid-Solid Transitions and Fusion of a Series of Eleven Primary Alkylamides by Differential Scanning Calorimetry |
| hsub | 86.00 ± 0.20 | kJ/mol | NIST Webbook |
| hsub | 86.00 ± 0.20 | kJ/mol | NIST Webbook |
| hvap | 41.50 | kJ/mol | Joback Method |
| log10ws | -0.46 | | Crippen Method |
| logp | 0.128 | | Crippen Method |
| mcvol | 78.770 | ml/mol | McGowan Method |
| pc | 4602.62 | kPa | Joback Method |
| rinpol | 923.00 | | NIST Webbook |
| rinpol | 923.00 | | NIST Webbook |
| tb | 491.20 | K | NIST Webbook |
| tc | 616.93 | K | Joback Method |

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|---|---|---|---|
| tf | 401.60 | K | Validation of the Vaporization Enthalpies of Some Simple Aliphatic Amides and Their Use in the Evaluation of the Vaporization Enthalpy of Valpromide and Valnoctamide |
| vc | 0.288 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 176.39 | J/mol×K | 516.91 | Joback Method |
| cpg | 183.71 | J/mol×K | 550.25 | Joback Method |
| cpg | 190.67 | J/mol×K | 583.59 | Joback Method |
| cpg | 152.24 | J/mol×K | 416.88 | Joback Method |
| cpg | 160.67 | J/mol×K | 450.22 | Joback Method |
| cpg | 168.72 | J/mol×K | 483.56 | Joback Method |
| cpg | 197.29 | J/mol×K | 616.93 | Joback Method |
| cps | 148.10 | J/mol×K | 298.15 | NIST Webbook |
| hfust | 19.20 | kJ/mol | 400.10 | NIST Webbook |
| hsubt | 86.00 | kJ/mol | 298.15 | NIST Webbook |
| hsubt | 86.10 ± 0.20 | kJ/mol | 293.50 | NIST Webbook |
| ssubt | 288.40 | J/mol×K | 298.15 | NIST Webbook |

# Sources

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|---|---|
| **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=C563837&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Validation of the Vaporization Enthalpies of Some Simple Aliphatic Amides and Their Use in the Evaluation of the Vaporization Enthalpy of Valpromide and Valnoctamide:** | https://www.doi.org/10.1021/je3012452 |
| **Heat Capacities and Enthalpies of Solid-Solid Transitions and Fusion of a Series of Eleven Primary Alkylamides by Differential Scanning Calorimetry:** | https://www.doi.org/10.1021/je700662a |

# Legend

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|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **cps:** | Solid phase heat capacity |
| **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 |
| **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 |
| **ssubt:** | Entropy of sublimation at a given temperature |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |