# Propanamide, N-isobutyl-2-methyl

**Inchi:** InChI=1S/C8H17NO/c1-6(2)5-9-8(10)7(3)4/h6-7H,5H2,1-4H3,(H,9,10)
**InchiKey:** MYLSYPDLABZVDQ-UHFFFAOYSA-N
**Formula:** C8H17NO
**SMILES:** CC(C)CNC(=O)C(C)C
**Mol. weight [g/mol]:** 143.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -27.93 | kJ/mol | Joback Method |
| hf | -278.12 | kJ/mol | Joback Method |
| hfus | 16.13 | kJ/mol | Joback Method |
| hvap | 45.81 | kJ/mol | Joback Method |
| log10ws | -1.65 | | Crippen Method |
| logp | 1.415 | | Crippen Method |
| mcvol | 135.130 | ml/mol | McGowan Method |
| pc | 2787.66 | kPa | Joback Method |
| rinpol | 1116.00 | | NIST Webbook |
| tb | 485.60 | K | Joback Method |
| tc | 672.00 | K | Joback Method |
| tf | 252.51 | K | Joback Method |
| vc | 0.512 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 302.58 | J/mol×K | 485.60 | Joback Method |
| cpg | 316.21 | J/mol×K | 516.67 | Joback Method |
| cpg | 329.23 | J/mol×K | 547.73 | Joback Method |
| cpg | 341.66 | J/mol×K | 578.80 | Joback Method |
| cpg | 353.50 | J/mol×K | 609.87 | Joback Method |
| cpg | 364.78 | J/mol×K | 640.93 | Joback Method |
| cpg | 375.50 | J/mol×K | 672.00 | Joback Method |

# 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=R50949&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |