

2-Propenamide, N-(1,1-dimethylethyl)-

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| Other names: | Acrylamide, N-tert-butyl- N-(1,1-dimethylethyl)-2-propenamide N-(tert-butyl)acrylamide N-t-Butyl-2-propenamide N-t-Butylacrylamide N-tert-butylacrylamide tert-Butylacrylamide |
| Inchi: | InChI=1S/C7H13NO/c1-5-6(9)8-7(2,3)4/h5H,1H2,2-4H3,(H,8,9) |
| InchiKey: | XFHJDMUEHUHAJW-UHFFFAOYSA-N |
| Formula: | C7H13NO |
| SMILES: | C=CC(=O)NC(C)(C)C |
| Mol. weight [g/mol]: | 127.18 |
| CAS: | 107-58-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|--|
| gf | 59.21 | kJ/mol | Joback Method |
| hf | -130.24 | kJ/mol | Joback Method |
| hfus | 21.57 | kJ/mol | Determination and Correlation of Solubility of N-tertbutylacrylamide in Seven Different Solvents at Temperatures between (279.15 and 353.15) K |
| hvap | 42.39 | kJ/mol | Joback Method |
| log10ws | -1.68 | | Crippen Method |
| logp | 1.087 | | Crippen Method |
| mcvol | 116.740 | ml/mol | McGowan Method |
| pc | 3254.14 | kPa | Joback Method |
| tb | 457.05 | K | Joback Method |
| tc | 652.95 | K | Joback Method |
| tf | 271.90 | K | Joback Method |
| vc | 0.439 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 245.35 | J/mol×K | 457.05 | Joback Method |
| cpg | 257.82 | J/mol×K | 489.70 | Joback Method |
| cpg | 269.55 | J/mol×K | 522.35 | Joback Method |
| cpg | 280.59 | J/mol×K | 555.00 | Joback Method |
| cpg | 290.97 | J/mol×K | 587.65 | Joback Method |
| cpg | 300.72 | J/mol×K | 620.30 | Joback Method |
| cpg | 309.87 | J/mol×K | 652.95 | Joback Method |

Sources

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|---|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Determination and Correlation of Solubility of N-tertbutylacrylamide in Several Different Solvents at Temperatures between (279.15 and 353.15) K: | https://www.doi.org/10.1021/acs.jced.5b00135 |
| 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=C107584&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|-----------------|---|
| 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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

Latest version available from:

<https://www.chemeo.com/cid/43-214-6/2-Propenamamide-N-1-1-dimethylethyl.pdf>

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