# 2-Acetylaminoheptane

**Other names:** Acetamide, N-(1-methylhexyl)-
**Inchi:** InChI=1S/C9H19NO/c1-4-5-6-7-8(2)10-9(3)11/h8H,4-7H2,1-3H3,(H,10,11)
**InchiKey:** XNHVITOEQJZLQB-UHFFFAOYSA-N
**Formula:** C9H19NO
**SMILES:** CCCCCC(C)NC(C)=O
**Mol. weight [g/mol]:** 157.25
**CAS:** 67282-69-3

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -17.07 | kJ/mol | Joback Method |
| hf | -293.48 | kJ/mol | Joback Method |
| hfus | 22.24 | kJ/mol | Joback Method |
| hvap | 48.42 | kJ/mol | Joback Method |
| log10ws | -2.67 | | Crippen Method |
| logp | 2.091 | | Crippen Method |
| mcvol | 149.220 | ml/mol | McGowan Method |
| pc | 2505.01 | kPa | Joback Method |
| rinpol | 1269.00 | | NIST Webbook |
| tb | 508.92 | K | Joback Method |
| tc | 689.58 | K | Joback Method |
| tf | 278.78 | K | Joback Method |
| vc | 0.575 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 347.35 | J/mol×K | 508.92 | Joback Method |
| cpg | 361.50 | J/mol×K | 539.03 | Joback Method |
| cpg | 375.03 | J/mol×K | 569.14 | Joback Method |
| cpg | 387.95 | J/mol×K | 599.25 | Joback Method |
| cpg | 400.29 | J/mol×K | 629.36 | Joback Method |
| cpg | 412.05 | J/mol×K | 659.47 | Joback Method |
| cpg | 423.26 | J/mol×K | 689.58 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C67282693&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |