# 6-nonynoic acid

**Inchi:** InChI=1S/C9H14O2/c1-2-3-4-5-6-7-8-9(10)11/h2,5-8H2,1H3,(H,10,11)
**InchiKey:** JYHVTTAHMRXBQX-UHFFFAOYSA-N
**Formula:** C9H14O2
**SMILES:** CCC#CCCCCC(=O)O
**Mol. weight [g/mol]:** 154.21
**CAS:** 56630-31-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.6681 | | Cheméo Relay (1.0) |
| gf | -38.04 | kJ/mol | Joback Method |
| hf | -311.87 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 27.88 | kJ/mol | Joback Method |
| hvap | 87.78 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.56 | eV | Cheméo Relay (1.0) |
| log10ws | -1.46 | | Cheméo Relay (1.0) |
| logp | 2.045 | | Crippen Method |
| mcvol | 136.510 | ml/mol | McGowan Method |
| pc | 3202.78 | kPa | Joback Method |
| tb | 518.67 | K | Cheméo Relay (1.0) |
| tc | 723.33 | K | Cheméo Relay (1.0) |
| tf | 302.27 | K | Cheméo Relay (1.0) |
| vc | 0.482 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 317.89 | J/mol×K | 560.37 | Joback Method |
| cpg | 328.66 | J/mol×K | 591.44 | Joback Method |
| cpg | 338.94 | J/mol×K | 622.52 | Joback Method |
| cpg | 348.75 | J/mol×K | 653.59 | Joback Method |
| cpg | 358.10 | J/mol×K | 684.67 | Joback Method |
| cpg | 367.00 | J/mol×K | 715.74 | Joback Method |
| cpg | 375.48 | J/mol×K | 746.82 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.57239e+01 |
| Coeff. B | -5.31769e+03 |
| Coeff. C | -1.02860e+02 |
| Temperature range (K), min. | 447.15 |
| Temperature range (K), max. | 613.15 |

# Sources

| | |
|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **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 |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |

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