# Pentan-2-one, 4-methyl-4-ethoxyamino

**Inchi:** InChI=1S/C8H17NO2/c1-5-11-9-8(3,4)6-7(2)10/h9H,5-6H2,1-4H3
**InchiKey:** VKMICPIUEABHKH-UHFFFAOYSA-N
**Formula:** C8H17NO2
**SMILES:** CCONC(C)(C)CC(C)=O
**Mol. weight [g/mol]:** 159.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -125.21 | kJ/mol | Joback Method |
| hf | -408.53 | kJ/mol | Joback Method |
| hfus | 16.95 | kJ/mol | Joback Method |
| hvap | 47.70 | kJ/mol | Joback Method |
| log10ws | -1.83 | | Crippen Method |
| logp | 1.285 | | Crippen Method |
| mcvol | 141.000 | ml/mol | McGowan Method |
| pc | 2746.90 | kPa | Joback Method |
| rinpol | 1007.00 | | NIST Webbook |
| tb | 505.67 | K | Joback Method |
| tc | 694.20 | K | Joback Method |
| tf | 307.16 | K | Joback Method |
| vc | 0.531 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 329.96 | J/mol×K | 505.67 | Joback Method |
| cpg | 343.63 | J/mol×K | 537.09 | Joback Method |
| cpg | 356.62 | J/mol×K | 568.51 | Joback Method |
| cpg | 368.97 | J/mol×K | 599.94 | Joback Method |
| cpg | 380.70 | J/mol×K | 631.36 | Joback Method |
| cpg | 391.81 | J/mol×K | 662.78 | Joback Method |
| cpg | 402.34 | J/mol×K | 694.20 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R315794&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |

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