# Azacyclononan-2-one

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|---|---|
| **Other names:** | 1H-Azonin-2(3H)-one, hexahydro-<br>2-Perhydroazoninone<br>2-azacyclononanone<br>2H-Azonin-2-one, octahydro-<br>8-Aminooctanoic acid lactam<br>8-Octanelactam<br>Capryllactam<br>Caprylolactam<br>NSC 59017<br>Octahydro-2H-azonin-2-one<br>Octamethylenimine, 2-oxo-<br>Octanoic acid, 8-amino-, lactam<br>cyclooctanone isooxime<br>«eta»-Capryllactam<br>«omega»-Caprylolactam<br>«omega»-Octalactam |
| **Inchi:** | InChI=1S/C8H15NO/c10-8-6-4-2-1-3-5-7-9-8/h1-7H2,(H,9,10) |
| **InchiKey:** | YDLSUFFXJYEVHW-UHFFFAOYSA-N |
| **Formula:** | C8H15NO |
| **SMILES:** | O=C1CCCCCCCN1 |
| **Mol. weight [g/mol]:** | 141.21 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.3960 | | Cheméo Relay (1.0) |
| gf | -22.54 | kJ/mol | Joback Method |
| hf | -321.42 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 10.04 | kJ/mol | Joback Method |
| hvap | 68.57 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.12 | eV | NIST Webbook |
| log10ws | -0.62 | | Cheméo Relay (1.0) |
| logp | 1.457 | | Crippen Method |
| mcvol | 124.270 | ml/mol | McGowan Method |
| pc | 3843.54 | kPa | Joback Method |
| tb | 554.82 | K | Cheméo Relay (1.0) |
| tc | 785.70 | K | Cheméo Relay (1.0) |
| tf | 353.83 | K | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 290.80 | J/mol×K | 535.84 | Joback Method |
| cpg | 311.06 | J/mol×K | 578.04 | Joback Method |
| cpg | 330.25 | J/mol×K | 620.24 | Joback Method |
| cpg | 348.31 | J/mol×K | 662.45 | Joback Method |
| cpg | 365.20 | J/mol×K | 704.65 | Joback Method |
| cpg | 380.86 | J/mol×K | 746.85 | Joback Method |
| cpg | 395.24 | J/mol×K | 789.05 | Joback Method |

# Sources

**Cheméo Relay (1.0, beta):**

| | |
|---|---|
| **Enthalpies of reaction of lanthanide trifluoroacetate trihydrate with 2-azacyclononanone to form lanthanide trifluoroacetate-tris 2-azacyclononanone:** | https://www.doi.org/10.1016/j.tca.2006.12.017 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C935308&Units=SI |
| **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):**

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |