# 2-n-Heptylcyclopentanone

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|---|---|
| **Other names:** | 2-Heptylcyclopentanone |
| | Cyclopentanone, 2-heptyl- |
| | Alismone |
| | Cyclopentanone, 2-n-heptyl- |
| | 2-Heptylcyclopentan-1-one |
| | «alpha»-Heptyl cyclopentanone |
| **Inchi:** | InChI=1S/C12H22O/c1-2-3-4-5-6-8-11-9-7-10-12(11)13/h11H,2-10H2,1H3 |
| **InchiKey:** | PJXHBTZLHITWFX-UHFFFAOYSA-N |
| **Formula:** | C12H22O |
| **SMILES:** | CCCCCCCC1CCCC1=O |
| **Mol. weight [g/mol]:** | 182.30 |
| **CAS:** | 137-03-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -35.88 | kJ/mol | Joback Method |
| hf | -368.23 | kJ/mol | Joback Method |
| hfus | 20.28 | kJ/mol | Joback Method |
| hvap | 46.81 | kJ/mol | Joback Method |
| log10ws | -3.78 | | Crippen Method |
| logp | 3.716 | | Crippen Method |
| mcvol | 170.650 | ml/mol | McGowan Method |
| pc | 2153.30 | kPa | Joback Method |
| rinpol | 1430.70 | | NIST Webbook |
| rinpol | 1430.70 | | NIST Webbook |
| tb | 557.06 | K | Joback Method |
| tc | 756.95 | K | Joback Method |
| tf | 304.12 | K | Joback Method |
| vc | 0.655 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 435.75 | J/mol×K | 557.06 | Joback Method |

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|---|---|---|---|---|
| cpg | 454.96 | J/mol×K | 590.38 | Joback Method |
| cpg | 473.27 | J/mol×K | 623.69 | Joback Method |
| cpg | 490.67 | J/mol×K | 657.01 | Joback Method |
| cpg | 507.20 | J/mol×K | 690.32 | Joback Method |
| cpg | 522.85 | J/mol×K | 723.64 | Joback Method |
| cpg | 537.65 | J/mol×K | 756.95 | Joback Method |

# Sources

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|---|---|
| **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=C137031&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **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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