# Cycloheptanol

**Other names:** SUBEROL
**Inchi:** InChI=1S/C7H14O/c8-7-5-3-1-2-4-6-7/h7-8H,1-6H2
**InchiKey:** QCRFMSUKWRQZEM-UHFFFAOYSA-N
**Formula:** C7H14O
**SMILES:** OC1CCCCCC1
**Mol. weight [g/mol]:** 114.19
**CAS:** 502-41-0

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -4362.00 ± 1.00 | kJ/mol | NIST Webbook |
| chl | -4429.20 | kJ/mol | NIST Webbook |
| gf | -116.41 | kJ/mol | Joback Method |
| hf | -291.88 | kJ/mol | Joback Method |
| hfus | 7.71 | kJ/mol | Joback Method |
| hvap | 48.46 | kJ/mol | Joback Method |
| log10ws | -0.88 | | Aqueous Solubility Prediction Method |
| log10ws | -0.88 | | Estimated Solubility Method |
| logp | 1.701 | | Crippen Method |
| mcvol | 104.500 | ml/mol | McGowan Method |
| pc | 4067.32 | kPa | Joback Method |
| rinpol | 1040.20 | | NIST Webbook |
| rinpol | 1022.00 | | NIST Webbook |
| rinpol | 1028.00 | | NIST Webbook |
| ripol | 1547.00 | | NIST Webbook |
| ripol | 1566.00 | | NIST Webbook |
| ripol | 1566.00 | | NIST Webbook |
| ripol | 1566.00 | | NIST Webbook |
| sl | 241.64 | J/mol×K | NIST Webbook |
| tb | 458.20 | K | NIST Webbook |
| tc | 675.73 | K | Joback Method |
| tf | 233.33 | K | Joback Method |
| tt | 280.30 ± 0.02 | K | NIST Webbook |
| vc | 0.371 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 230.00 | J/mol×K | 475.56 | Joback Method |
| cpg | 308.33 | J/mol×K | 675.73 | Joback Method |
| cpg | 244.83 | J/mol×K | 508.92 | Joback Method |
| cpg | 258.94 | J/mol×K | 542.28 | Joback Method |
| cpg | 272.33 | J/mol×K | 575.64 | Joback Method |
| cpg | 285.01 | J/mol×K | 609.00 | Joback Method |
| cpg | 297.01 | J/mol×K | 642.37 | Joback Method |
| cpl | 250.22 | J/mol×K | 298.15 | NIST Webbook |
| cpl | 244.30 | J/mol×K | 298.00 | NIST Webbook |
| cps | 198.10 | J/mol×K | 264.00 | Heat capacities of selected cycloalcohols |
| cps | 199.80 | J/mol×K | 266.00 | Heat capacities of selected cycloalcohols |
| cps | 199.80 | J/mol×K | 266.00 | Heat capacities of selected cycloalcohols |
| cps | 198.00 | J/mol×K | 264.00 | Heat capacities of selected cycloalcohols |
| cps | 196.50 | J/mol×K | 262.00 | Heat capacities of selected cycloalcohols |
| cps | 196.40 | J/mol×K | 262.00 | Heat capacities of selected cycloalcohols |
| cps | 195.30 | J/mol×K | 260.59 | Heat capacities of selected cycloalcohols |
| cps | 201.80 | J/mol×K | 268.00 | Heat capacities of selected cycloalcohols |
| cps | 201.70 | J/mol×K | 268.00 | Heat capacities of selected cycloalcohols |
| cps | 204.00 | J/mol×K | 270.00 | Heat capacities of selected cycloalcohols |
| cps | 204.00 | J/mol×K | 270.00 | Heat capacities of selected cycloalcohols |
| cps | 205.20 | J/mol×K | 271.34 | Heat capacities of selected cycloalcohols |

| | | | | |
|---|---|---|---|---|
| cps | 205.40 | J/mol×K | 271.43 | Heat capacities of selected cycloalcohols |
| cps | 195.40 | J/mol×K | 260.73 | Heat capacities of selected cycloalcohols |
| dvisc | 0.0044230 | Pa×s | 314.07 | Joback Method |
| dvisc | 0.0006163 | Pa×s | 394.82 | Joback Method |
| dvisc | 0.0003026 | Pa×s | 435.19 | Joback Method |
| dvisc | 0.0014757 | Pa×s | 354.44 | Joback Method |
| dvisc | 0.1241815 | Pa×s | 233.33 | Joback Method |
| dvisc | 0.0183260 | Pa×s | 273.70 | Joback Method |
| dvisc | 0.0001677 | Pa×s | 475.56 | Joback Method |
| hfust | 2.93 | kJ/mol | 172.20 | NIST Webbook |
| hfust | 0.88 | kJ/mol | 258.40 | NIST Webbook |
| hfust | 1.60 | kJ/mol | 280.30 | NIST Webbook |
| hfust | 0.55 | kJ/mol | 227.30 | NIST Webbook |
| hfust | 1.51 | kJ/mol | 278.30 | NIST Webbook |
| hfust | 1.60 | kJ/mol | 280.30 | NIST Webbook |
| hvapt | 64.70 | kJ/mol | 303.50 | NIST Webbook |
| hvapt | 67.40 | kJ/mol | 302.50 | NIST Webbook |
| pvap | 7.50e-03 | kPa | 284.67 | Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols |
| pvap | 0.07 | kPa | 308.15 | Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols |
| pvap | 0.08 | kPa | 310.11 | Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols |

| | | | | | |
|---|---|---|---|---|---|
| pvap | 0.16 | kPa | 319.51 | Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols | |
| pvap | 0.06 | kPa | 307.00 | Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols | |
| pvap | 0.04 | kPa | 303.37 | Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols | |
| pvap | 0.03 | kPa | 298.44 | Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols | |
| pvap | 0.03 | kPa | 298.28 | Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols | |

| | | | | | |
|---|---|---|---|---|---|
| pvap | 0.03 | kPa | 298.23 | Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols | |
| pvap | 0.02 | kPa | 293.86 | Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols | |
| pvap | 0.12 | kPa | 315.14 | Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols | |
| pvap | 7.10e-03 | kPa | 284.35 | Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols | |
| pvap | 0.02 | kPa | 293.72 | Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols | |

| | | | | |
|---|---|---|---|---|
| pvap | 0.02 | kPa | 292.50 | Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols |
| pvap | 0.01 | kPa | 288.22 | Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols |
| pvap | 0.02 | kPa | 293.73 | Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols |
| pvap | 0.18 | kPa | 320.88 | Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols |
| sfust | 5.72 | J/mol×K | 280.30 | NIST Webbook |
| sfust | 16.98 | J/mol×K | 172.20 | NIST Webbook |
| sfust | 2.44 | J/mol×K | 227.30 | NIST Webbook |
| sfust | 3.39 | J/mol×K | 258.40 | NIST Webbook |
| srf | 0.02 | N/m | 323.15 | Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol |
| srf | 0.03 | N/m | 298.15 | Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol |

| | | | | |
|---|---|---|---|---|
| srf | 0.03 | N/m | 293.15 | Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol |
| srf | 0.03 | N/m | 318.15 | Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol |
| srf | 0.03 | N/m | 313.15 | Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol |
| srf | 0.03 | N/m | 308.15 | Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol |
| srf | 0.03 | N/m | 303.15 | Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | -2.66915e+01 |
| Coeff. B | -5.85520e+03 |
| Coeff. C | 7.60167e+00 |
| Coeff. D | -6.45886e-06 |
| Temperature range (K), min. | 284.15 |
| Temperature range (K), max. | 323.15 |

# Sources

| | |
|---|---|
| **KDB:** | https://www.cheric.org/files/research/kdb/mol/mol900.mol |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Surface Tensions of Dilute Solutions of Cycloheptanol in Ethylene Glycol:** | https://www.doi.org/10.1021/je050055m |
| **Vapor Pressure and its Temperature Dependence of 28 Organic Compounds:** | https://www.doi.org/10.1021/acs.jced.6b00576 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols:** | |

| | |
|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=900 |
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C502410&Units=SI |
| **Heat capacities of selected cycloalcohols:** | https://www.doi.org/10.1016/j.tca.2014.10.002 |

# Legend

| | |
|---|---|
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase heat capacity |
| **cps:** | Solid phase heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **sfust:** | Entropy of fusion at a given temperature |
| **sl:** | Liquid phase molar entropy at standard conditions |
| **srf:** | Surface Tension |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **tt:** | Triple Point Temperature |
| **vc:** | Critical Volume |