# cyclohexapentylose

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|---|---|
| **Other names:** | .alpha.-cyclodextrin<br>cyclohexaamylose<br>«alpha»-Cyclodextrin |
| **Inchi:** | InChI=1S/C36H60O30/c37-1-7-25-13(43)19(49)31(55-7)62-26-8(2-38)57-33(21(51)15(26 |
| **InchiKey:** | HFHDHCJBZVLPGP-OQDZSFIYSA-N |
| **Formula:** | C36H60O30 |
| **SMILES:** | OCC1OC2OC3C(CO)OC(OC4C(CO)OC(OC5C(CO)OC(OC6C(CO)OC(OC7C(CO)OC(O |
| **Mol. weight [g/mol]:** | 972.84 |
| **CAS:** | 10016-20-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -3250.14 | kJ/mol | Joback Method |
| hf | -5198.09 | kJ/mol | Joback Method |
| hfus | 225.81 | kJ/mol | Joback Method |
| hvap | 445.97 | kJ/mol | Joback Method |
| log10ws | 3.73 | | Crippen Method |
| logp | -13.055 | | Crippen Method |
| mcvol | 618.180 | ml/mol | McGowan Method |
| pc | 1665.97 | kPa | Joback Method |
| tb | 3035.16 | K | Joback Method |
| tf | 1863.22 | K | Joback Method |
| vc | 2.154 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | -4554.46 | J/mol×K | 3035.16 | Joback Method |
| cpg | 2567.48 | J/mol×K | 1233.51 | Joback Method |
| cpg | 1181.50 | J/mol×K | 332.68 | Joback Method |
| cpg | 790.29 | J/mol×K | 2134.33 | Joback Method |

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|---|---|---|---|---|
| cps | 1201.50 | J/mol×K | 308.15 | Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides |
| cps | 1212.60 | J/mol×K | 313.15 | Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides |
| cps | 1230.20 | J/mol×K | 318.15 | Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides |
| cps | 1259.30 | J/mol×K | 323.15 | Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides |
| cps | 1282.60 | J/mol×K | 328.15 | Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides |
| cps | 1164.10 | J/mol×K | 303.15 | Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides |
| cps | 1335.30 | J/mol×K | 338.15 | Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides |
| cps | 1364.60 | J/mol×K | 343.15 | Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides |
| cps | 1401.60 | J/mol×K | 348.15 | Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides |

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|---|---|---|---|---|---|
| cps | 1150.00 | J/mol×K | 298.15 | Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides | |
| cps | 1502.70 | J/mol×K | 358.15 | Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides | |
| cps | 1153.00 | J/mol×K | 298.15 | NIST Webbook | |
| cps | 1113.20 | J/mol×K | 293.15 | Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides | |
| cps | 1305.30 | J/mol×K | 333.15 | Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides | |
| cps | 1442.60 | J/mol×K | 353.15 | Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides | |
| cps | 1074.60 | J/mol×K | 288.15 | Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides | |
| dvisc | 0.0000000 | Pa×s | 2449.19 | Joback Method | |
| dvisc | 0.0000000 | Pa×s | 2839.84 | Joback Method | |
| dvisc | 0.0000000 | Pa×s | 3035.16 | Joback Method | |
| dvisc | 0.0000000 | Pa×s | 2253.87 | Joback Method | |
| dvisc | 0.0000000 | Pa×s | 2058.54 | Joback Method | |
| dvisc | 0.0000000 | Pa×s | 1863.22 | Joback Method | |
| dvisc | 0.0000000 | Pa×s | 2644.51 | Joback Method | |

# Sources

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|---|---|
| **Effect of different excipients on aqueous solubility of ketoconazole: Thermodynamic study:** | https://www.doi.org/10.1016/j.tca.2016.08.010 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides:** | https://www.doi.org/10.1016/j.jct.2008.08.007 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Binary Mutual Diffusion Coefficients of Aqueous Solutions of r-Cyclodextrin, 2-Hydroxypropyl-r-cyclodextrin, and alpha-cyclodextrin at 298.15 K:** | https://www.doi.org/10.1021/je060474z |
| **Thermodynamic studies of drug interactions in binary aqueous solutions (298.15 to 312.15) Volumetric approach: Interactions of some local anesthetical drugs with alpha-cyclodextrin in aqueous solutions at 298.15 K:** | https://www.doi.org/10.1016/j.jct.2013.09.003 |
| **Limiting diffusion coefficients of sodium octanoate and octanoic acid in aqueous solutions of alpha-cyclodextrin at 298.15 K:** | https://www.doi.org/10.1016/j.jct.2015.11.013 |
| **Hydrochloride/Mideodrine Hydrochloride + Alpha-Cyclodextrin + H2O Systems: Measurement and correlation of solubilities of the poorlywater-soluble pharmaceutical compound etodolac by addition of cosolvents:** | https://www.doi.org/10.1016/j.jct.2016.12.023 |
| **Activity Coefficient Studies in Ternary Aqueous Solutions at 298.15 K: H2O + Potassium Acetate and H2O + 18-Crown-6 + Hydroquinone Systems:** | https://www.doi.org/10.1016/j.jct.2016.06.008 |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C10016203&Units=SI |
| **Effect of presence of alpha-cyclodextrin and beta-cyclodextrin on solution behavior of sulfathiazole at different temperatures: Thermodynamic and spectroscopic studies:** | https://www.doi.org/10.1016/j.jct.2017.12.017 |
| **Mcvol Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **alpha-cyclodextrin hexahydrate dehydration of alpha-cyclodextrin hexahydrate:** | https://www.doi.org/10.1016/j.fluid.2013.05.025 |
| **Hydrochloride/Mideodrine Hydrochloride + Alpha-Cyclodextrin + H2O Systems: Measurement and correlation of solubilities of the poorlywater-soluble pharmaceutical compound etodolac by addition of cosolvents:** | https://www.doi.org/10.1021/je800307g |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C10016203&Units=SI |
| **Effect of presence of alpha-cyclodextrin and beta-cyclodextrin on solution behavior of sulfathiazole at different temperatures: Thermodynamic and spectroscopic studies:** | https://www.doi.org/10.1016/j.jct.2017.12.017 |


# Legend

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|---|---|
| **cpg:** | Ideal gas 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 |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |


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