# Cyclohexanol, 1-ethynyl-

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|---|---|
| **Other names:** | (1-Hydroxycyclohexyl)ethyne |
| | 1-Ethynyl-1-cyclohexanol |
| | 1-Ethynyl-1-hydroxycyclohexane |
| | 1-Ethynylcyclohexan-1-ol |
| | 1-Ethynylcyclohexanol |
| | Ethynylcyclohexanol |
| | 1-Hydroxy-1-ethynylcyclohexane |
| **Inchi:** | InChI=1S/C8H12O/c1-2-8(9)6-4-3-5-7-8/h1,9H,3-7H2 |
| **InchiKey:** | QYLFHLNFIHBCPR-UHFFFAOYSA-N |
| **Formula:** | C8H12O |
| **SMILES:** | C#CC1(O)CCCCC1 |
| **Mol. weight [g/mol]:** | 124.18 |
| **CAS:** | 78-27-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 121.69 | kJ/mol | Joback Method |
| hf | 0.78 | kJ/mol | Joback Method |
| hfus | 9.08 | kJ/mol | Joback Method |
| hvap | 49.22 | kJ/mol | Joback Method |
| ie | 10.60 | eV | NIST Webbook |
| log10ws | -2.24 | | Crippen Method |
| logp | 1.315 | | Crippen Method |
| mcvol | 109.990 | ml/mol | McGowan Method |
| pc | 4468.24 | kPa | Joback Method |
| tb | 453.20 | K | NIST Webbook |
| tc | 697.51 | K | Joback Method |
| tf | 305.00 ± 3.00 | K | NIST Webbook |
| vc | 0.396 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 241.68 | J/mol×K | 484.53 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 255.15 | J/mol×K | 520.03 | Joback Method |
| cpg | 267.63 | J/mol×K | 555.52 | Joback Method |
| cpg | 279.22 | J/mol×K | 591.02 | Joback Method |
| cpg | 290.04 | J/mol×K | 626.52 | Joback Method |
| cpg | 300.19 | J/mol×K | 662.01 | Joback Method |
| cpg | 309.80 | J/mol×K | 697.51 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 347.00 | K | 1.60 | NIST Webbook |

# Sources

**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=C78273&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

# 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
**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
**tbrp:** Boiling point at reduced pressure
**tc:** Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume