# Cyclohexylphenylacetonitrile

**Other names:** «alpha»-Cyclohexylphenylacetonitrile
Benzeneacetonitrile, «alpha»-cyclohexyl-
**Inchi:** InChI=1S/C14H17N/c15-11-14(12-7-3-1-4-8-12)13-9-5-2-6-10-13/h1,3-4,7-8,13-14H,2,5-
**InchiKey:** IZSWBXTYTALSOZ-UHFFFAOYSA-N
**Formula:** C14H17N
**SMILES:** N#CC(c1ccccc1)C1CCCCC1
**Mol. weight [g/mol]:** 199.29
**CAS:** 3893-23-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 334.60 | kJ/mol | Joback Method |
| hf | 118.16 | kJ/mol | Joback Method |
| hfus | 15.88 | kJ/mol | Joback Method |
| hvap | 59.55 | kJ/mol | Joback Method |
| log10ws | -4.27 | | Crippen Method |
| logp | 3.874 | | Crippen Method |
| mcvol | 174.880 | ml/mol | McGowan Method |
| pc | 2395.87 | kPa | Joback Method |
| tb | 667.59 | K | Joback Method |
| tc | 917.77 | K | Joback Method |
| tf | 331.33 | K | Joback Method |
| vc | 0.664 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 473.87 | J/mol×K | 667.59 | Joback Method |
| cpg | 492.51 | J/mol×K | 709.29 | Joback Method |
| cpg | 509.64 | J/mol×K | 750.98 | Joback Method |
| cpg | 525.36 | J/mol×K | 792.68 | Joback Method |
| cpg | 539.73 | J/mol×K | 834.38 | Joback Method |
| cpg | 552.85 | J/mol×K | 876.07 | Joback Method |
| cpg | 564.78 | J/mol×K | 917.77 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **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=C3893230&Units=SI |

# 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 |
| **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 |
| **vc:** | Critical Volume |