# Phenyl cyclohexyl ketone

| | |
|---|---|
| **Other names:** | Methanone, cyclohexylphenyl- |
| | Ketone, cyclohexyl phenyl |
| | Benzophenone, 1,2,3,4,5,6-hexahydro- |
| | Benzoyl cyclohexane |
| | Cyclohexyl phenyl ketone |
| | USAF KF-3 |
| **Inchi:** | InChI=1S/C13H16O/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1,3-4,7-8,12H,2,5-6,9-10 |
| **InchiKey:** | BMFYCFSWWDXEPB-UHFFFAOYSA-N |
| **Formula:** | C13H16O |
| **SMILES:** | O=C(c1ccccc1)C1CCCCC1 |
| **Mol. weight [g/mol]:** | 188.27 |
| **CAS:** | 712-50-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 66.52 | kJ/mol | Joback Method |
| hf | -133.38 | kJ/mol | Joback Method |
| hfus | 16.90 | kJ/mol | Joback Method |
| hvap | 53.98 | kJ/mol | Joback Method |
| log10ws | -3.88 | | Crippen Method |
| logp | 3.450 | | Crippen Method |
| mcvol | 160.980 | ml/mol | McGowan Method |
| pc | 2868.87 | kPa | Joback Method |
| rinpol | 1608.00 | | NIST Webbook |
| tb | 596.94 | K | Joback Method |
| tc | 840.91 | K | Joback Method |
| tf | 332.50 ± 0.50 | K | NIST Webbook |
| vc | 0.595 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 406.71 | J/mol×K | 596.94 | Joback Method |
| cpg | 426.59 | J/mol×K | 637.60 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 444.96 | J/mol×K | 678.26 | Joback Method |
| cpg | 461.91 | J/mol×K | 718.92 | Joback Method |
| cpg | 477.50 | J/mol×K | 759.58 | Joback Method |
| cpg | 491.80 | J/mol×K | 800.24 | Joback Method |
| cpg | 504.88 | J/mol×K | 840.91 | Joback Method |
| dvisc | 0.0037215 | Pa×s | 320.00 | Joback Method |
| dvisc | 0.0017342 | Pa×s | 366.16 | Joback Method |
| dvisc | 0.0009588 | Pa×s | 412.31 | Joback Method |
| dvisc | 0.0005973 | Pa×s | 458.47 | Joback Method |
| dvisc | 0.0004057 | Pa×s | 504.63 | Joback Method |
| dvisc | 0.0002940 | Pa×s | 550.78 | Joback Method |
| dvisc | 0.0002240 | Pa×s | 596.94 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 437.70 | K | 2.40 | NIST Webbook |
| tbrp | 428.00 ± 2.00 | K | 2.00 | NIST Webbook |
| tbrp | 437.50 ± 0.50 | K | 2.40 | NIST Webbook |

# Sources

**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=C712505&Units=SI

# Legend

**cpg:** Ideal gas 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |