# 3-Buten-2-one, 4-(4-chlorophenyl)-

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|---|---|
| **Other names:** | 4-Chlorobenzalacetone |
| | 3-Buten-2-one, 4-(p-chlorophenyl)- |
| | (p-Chlorobenzylidene)acetone |
| | (4-Chlorobenzylidene)acetone |
| | 4-(4-Chlorophenyl)-3-buten-2-one |
| | 1-(4-Chlorophenyl)-1-buten-3-one |
| | p-Chlorobenzalacetone |
| | 4-(4-Chlorophenyl)-but-3-en-2-one |
| | 4-[p-Chlorophenyl]-3-butene-2-one |
| **Inchi:** | InChI=1S/C10H9ClO/c1-8(12)2-3-9-4-6-10(11)7-5-9/h2-7H,1H3/b3-2+ |
| **InchiKey:** | UUKRKWJGNHNTRG-NSCUHMNNSA-N |
| **Formula:** | C10H9ClO |
| **SMILES:** | CC(=O)C=Cc1ccc(Cl)cc1 |
| **Mol. weight [g/mol]:** | 180.63 |
| **CAS:** | 3160-40-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 75.47 | kJ/mol | Joback Method |
| hf | -35.77 | kJ/mol | Joback Method |
| hfus | 21.31 | kJ/mol | Joback Method |
| hvap | 51.88 | kJ/mol | Joback Method |
| ie | 8.70 | eV | NIST Webbook |
| log10ws | -3.10 | | Crippen Method |
| logp | 2.942 | | Crippen Method |
| mcvol | 137.510 | ml/mol | McGowan Method |
| pc | 3142.03 | kPa | Joback Method |
| tb | 555.32 | K | Joback Method |
| tc | 786.44 | K | Joback Method |
| tf | 316.17 | K | Joback Method |
| vc | 0.522 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 283.35 | J/mol×K | 555.32 | Joback Method |
| cpg | 295.44 | J/mol×K | 593.84 | Joback Method |
| cpg | 306.65 | J/mol×K | 632.36 | Joback Method |
| cpg | 317.05 | J/mol×K | 670.88 | Joback Method |
| cpg | 326.69 | J/mol×K | 709.40 | Joback Method |
| cpg | 335.63 | J/mol×K | 747.92 | Joback Method |
| cpg | 343.91 | J/mol×K | 786.44 | Joback Method |
| dvisc | 0.0020142 | Pa×s | 316.17 | Joback Method |
| dvisc | 0.0011317 | Pa×s | 356.03 | Joback Method |
| dvisc | 0.0007142 | Pa×s | 395.89 | Joback Method |
| dvisc | 0.0004903 | Pa×s | 435.75 | Joback Method |
| dvisc | 0.0003585 | Pa×s | 475.60 | Joback Method |
| dvisc | 0.0002751 | Pa×s | 515.46 | Joback Method |
| dvisc | 0.0002193 | Pa×s | 555.32 | Joback Method |

# Sources

**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=C3160405&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# 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
**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

| | |
|---|---|
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |