# 4-Butylcyclopenten-3-one

**Inchi:** InChI=1S/C9H14O/c1-2-3-5-8-6-4-7-9(8)10/h4,7-8H,2-3,5-6H2,1H3
**InchiKey:** TZIXJRCVLIIIEA-UHFFFAOYSA-N
**Formula:** C9H14O
**SMILES:** CCCCC1CC=CC1=O
**Mol. weight [g/mol]:** 138.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -31.18 | kJ/mol | Joback Method |
| hf | -248.53 | kJ/mol | Joback Method |
| hfus | 13.73 | kJ/mol | Joback Method |
| hvap | 40.42 | kJ/mol | Joback Method |
| log10ws | -2.38 | | Crippen Method |
| logp | 2.322 | | Crippen Method |
| mcvol | 124.080 | ml/mol | McGowan Method |
| pc | 2982.79 | kPa | Joback Method |
| ripol | 1599.00 | | NIST Webbook |
| ripol | 1599.00 | | NIST Webbook |
| tb | 487.58 | K | Joback Method |
| tc | 698.55 | K | Joback Method |
| tf | 271.07 | K | Joback Method |
| vc | 0.473 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 275.12 | J/mol×K | 487.58 | Joback Method |
| cpg | 290.82 | J/mol×K | 522.74 | Joback Method |
| cpg | 305.80 | J/mol×K | 557.90 | Joback Method |
| cpg | 320.05 | J/mol×K | 593.07 | Joback Method |
| cpg | 333.59 | J/mol×K | 628.23 | Joback Method |
| cpg | 346.42 | J/mol×K | 663.39 | Joback Method |
| cpg | 358.55 | J/mol×K | 698.55 | 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=R548251&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |