# 3-BUTYL-2-HYDROXY-2-CYCLOPENTEN-1-ONE

**Other names:** 2-Cyclopenten-1-one, 3-butyl-2-hydroxy
**Inchi:** InChI=1S/C9H14O2/c1-2-3-4-7-5-6-8(10)9(7)11/h11H,2-6H2,1H3
**InchiKey:** UJTQSQADRGAFHN-UHFFFAOYSA-N
**Formula:** C9H14O2
**SMILES:** CCCCC1=C(O)C(=O)CC1
**Mol. weight [g/mol]:** 154.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 15.97 | kJ/mol | Joback Method |
| logp | 2.352 | | Crippen Method |
| mcvol | 129.950 | ml/mol | McGowan Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 328.33 | J/mol×K | 594.39 | Joback Method |
| cpg | 340.69 | J/mol×K | 627.61 | Joback Method |
| cpg | 352.48 | J/mol×K | 660.82 | Joback Method |
| cpg | 363.69 | J/mol×K | 694.04 | Joback Method |
| cpg | 374.34 | J/mol×K | 727.26 | Joback Method |
| cpg | 384.42 | J/mol×K | 760.47 | Joback Method |
| cpg | 393.94 | J/mol×K | 793.69 | Joback Method |

## Sources

**Cheméo Relay (1.0, beta):**
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C29798729&Units=SI
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Cheméo Relay (1.0):**

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |