# 1,2,4-Cyclopentanetrione, 3-butyl-

**Other names:** 3-Butyl-1,2,4-cyclopentanetrione
**Inchi:** InChI=1S/C9H12O3/c1-2-3-4-6-7(10)5-8(11)9(6)12/h6H,2-5H2,1H3
**InchiKey:** HMFXLRRRGHKBCH-UHFFFAOYSA-N
**Formula:** C9H12O3
**SMILES:** CCCCC1C(=O)CC(=O)C1=O
**Mol. weight [g/mol]:** 168.19
**CAS:** 46005-09-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -306.32 | kJ/mol | Joback Method |
| hf | -581.71 | kJ/mol | Joback Method |
| hfus | 11.53 | kJ/mol | Joback Method |
| hvap | 48.63 | kJ/mol | Joback Method |
| log10ws | -1.08 | | Crippen Method |
| logp | 0.904 | | Crippen Method |
| mcvol | 131.520 | ml/mol | McGowan Method |
| pc | 3096.73 | kPa | Joback Method |
| rinpol | 1486.00 | | NIST Webbook |
| rinpol | 1486.00 | | NIST Webbook |
| tb | 624.06 | K | Joback Method |
| tc | 861.71 | K | Joback Method |
| tf | 406.75 | K | Joback Method |
| vc | 0.501 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 351.14 | J/mol×K | 624.06 | Joback Method |
| cpg | 367.42 | J/mol×K | 663.67 | Joback Method |
| cpg | 382.87 | J/mol×K | 703.28 | Joback Method |
| cpg | 397.40 | J/mol×K | 742.89 | Joback Method |
| cpg | 410.95 | J/mol×K | 782.50 | Joback Method |
| cpg | 423.43 | J/mol×K | 822.11 | Joback Method |

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|---|---|---|---|---|
| cpg | 434.77 | J/mol×K | 861.71 | Joback Method |

# Sources

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|---|---|
| **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=C46005098&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |