# 1-Butanol, 3-methyl-, carbonate (2:1)

**Other names:** Di-iso-amyl carbonate
diisopentyl carbonate
**Inchi:** InChI=1S/C11H22O3/c1-9(2)5-7-13-11(12)14-8-6-10(3)4/h9-10H,5-8H2,1-4H3
**InchiKey:** DWWPOAYNAWHBKI-UHFFFAOYSA-N
**Formula:** C11H22O3
**SMILES:** CC(C)CCOC(=O)OCCC(C)C
**Mol. weight [g/mol]:** 202.29
**CAS:** 2050-95-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -302.06 | kJ/mol | Joback Method |
| hf | -657.95 | kJ/mol | Joback Method |
| hfus | 21.18 | kJ/mol | Joback Method |
| hvap | 50.87 | kJ/mol | Joback Method |
| log10ws | -2.87 | | Crippen Method |
| logp | 3.232 | | Crippen Method |
| mcvol | 179.160 | ml/mol | McGowan Method |
| pc | 2012.70 | kPa | Joback Method |
| tb | 505.35 ± 0.40 | K | NIST Webbook |
| tc | 725.84 | K | Joback Method |
| tf | 278.12 | K | Joback Method |
| vc | 0.681 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 442.83 | J/mol×K | 548.91 | Joback Method |
| cpg | 458.24 | J/mol×K | 578.40 | Joback Method |
| cpg | 473.06 | J/mol×K | 607.89 | Joback Method |
| cpg | 487.29 | J/mol×K | 637.38 | Joback Method |
| cpg | 500.93 | J/mol×K | 666.86 | Joback Method |
| cpg | 513.98 | J/mol×K | 696.35 | Joback Method |
| cpg | 526.44 | J/mol×K | 725.84 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0043534 | Pa×s | 278.12 | Joback Method |
| dvisc | 0.0016670 | Pa×s | 323.25 | Joback Method |
| dvisc | 0.0008076 | Pa×s | 368.38 | Joback Method |
| dvisc | 0.0004583 | Pa×s | 413.52 | Joback Method |
| dvisc | 0.0002908 | Pa×s | 458.65 | Joback Method |
| dvisc | 0.0002001 | Pa×s | 503.78 | Joback Method |
| dvisc | 0.0001465 | Pa×s | 548.91 | Joback Method |

# Sources

| | |
|---|---|
| **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=C2050955&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 |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |