# 2-Butyne-1,4-diol, diacetate

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|---|---|
| **Other names:** | Butynediol diacetate |
| | 1,4-Diacetoxy-2-butyne |
| | 2-Butynediol-1,4-diacetate |
| | but-2-yne-1,4-diyl diacetate |
| **Inchi:** | InChI=1S/C8H10O4/c1-7(9)11-5-3-4-6-12-8(2)10/h5-6H2,1-2H3 |
| **InchiKey:** | TVIMIQVBDDNCCR-UHFFFAOYSA-N |
| **Formula:** | C8H10O4 |
| **SMILES:** | CC(=O)OCC#CCOC(C)=O |
| **Mol. weight [g/mol]:** | 170.16 |
| **CAS:** | 1573-17-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -248.56 | kJ/mol | Joback Method |
| hf | -425.75 | kJ/mol | Joback Method |
| hfus | 25.17 | kJ/mol | Joback Method |
| hvap | 53.87 | kJ/mol | Joback Method |
| log10ws | -0.69 | | Crippen Method |
| logp | 0.116 | | Crippen Method |
| mcvol | 129.860 | ml/mol | McGowan Method |
| pc | 3325.84 | kPa | Joback Method |
| tb | 544.02 | K | Joback Method |
| tc | 750.31 | K | Joback Method |
| tf | 430.34 | K | Joback Method |
| vc | 0.493 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 285.58 | J/mol×K | 544.02 | Joback Method |
| cpg | 296.01 | J/mol×K | 578.40 | Joback Method |
| cpg | 306.03 | J/mol×K | 612.78 | Joback Method |
| cpg | 315.63 | J/mol×K | 647.17 | Joback Method |
| cpg | 324.79 | J/mol×K | 681.55 | Joback Method |

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|---|---|---|---|---|
| cpg | 333.49 | J/mol×K | 715.93 | Joback Method |
| cpg | 341.73 | J/mol×K | 750.31 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 395.70 | K | 1.30 | NIST Webbook |

# 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=C1573177&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |