# 1-Propyne, 3,3'-oxybis-

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|---|---|
| **Other names:** | Dipropargyl ether |
| | 2-Propynyl ether |
| | Dipropargyl oxide |
| | Propargyl ether |
| | (HC«equiv»CCH2)2O |
| | Di(2-propynyl) ether |
| | Bis(2-propynyl) ether |
| **Inchi:** | InChI=1S/C6H6O/c1-3-5-7-6-4-2/h1-2H,5-6H2 |
| **InchiKey:** | HRDCVMSNCBAMAM-UHFFFAOYSA-N |
| **Formula:** | C6H6O |
| **SMILES:** | C#CCOCC#C |
| **Mol. weight [g/mol]:** | 94.11 |
| **CAS:** | 6921-27-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 783.90 | kJ/mol | NIST Webbook |
| basg | 756.50 | kJ/mol | NIST Webbook |
| gf | 340.78 | kJ/mol | Joback Method |
| hf | 284.41 | kJ/mol | Joback Method |
| hfus | 18.43 | kJ/mol | Joback Method |
| hvap | 31.08 | kJ/mol | Joback Method |
| log10ws | -1.01 | | Crippen Method |
| logp | 0.269 | | Crippen Method |
| mcvol | 84.070 | ml/mol | McGowan Method |
| pc | 4356.87 | kPa | Joback Method |
| tb | 339.34 | K | Joback Method |
| tc | 528.84 | K | Joback Method |
| tf | 273.55 | K | Joback Method |
| vc | 0.314 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

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|---|---|---|---|---|
| cpg | 140.55 | J/mol×K | 339.34 | Joback Method |
| cpg | 147.14 | J/mol×K | 370.92 | Joback Method |
| cpg | 153.45 | J/mol×K | 402.51 | Joback Method |
| cpg | 159.50 | J/mol×K | 434.09 | Joback Method |
| cpg | 165.29 | J/mol×K | 465.68 | Joback Method |
| cpg | 170.83 | J/mol×K | 497.26 | Joback Method |
| cpg | 176.13 | J/mol×K | 528.84 | 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=C6921273&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **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 |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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