

Methyl propargyl ether

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| Other names: | HC«equiv»CCH2OCH3 1-Propyne, 3-methoxy- Ether, methyl 2-propynyl 3-Methoxypropyne 3-Methoxy-1-propyne Propargyl methyl ether Methyl 2-propynyl ether 3-Methoxyprop-1-yne |
| Inchi: | InChI=1S/C4H6O/c1-3-4-5-2/h1H,4H2,2H3 |
| InchiKey: | YACFFSVYSPMSGS-UHFFFAOYSA-N |
| Formula: | C4H6O |
| SMILES: | C#CCOC |
| Mol. weight [g/mol]: | 70.09 |
| CAS: | 627-41-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 100.87 | kJ/mol | Joback Method |
| hf | 33.79 | kJ/mol | Joback Method |
| hfus | 10.28 | kJ/mol | Joback Method |
| hvap | 26.77 | kJ/mol | Joback Method |
| ie | 9.78 | eV | NIST Webbook |
| log10ws | -0.38 | | Crippen Method |
| logp | 0.266 | | Crippen Method |
| mcvol | 64.490 | ml/mol | McGowan Method |
| pc | 4621.41 | kPa | Joback Method |
| tb | 334.70 | K | NIST Webbook |
| tc | 478.93 | K | Joback Method |
| tf | 204.04 | K | Joback Method |
| vc | 0.239 | m3/kmol | Joback Method |

Temperature Dependent Properties

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

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|-----|--------|---------|--------|---------------|
| cpg | 100.08 | J/mol×K | 303.46 | Joback Method |
| cpg | 105.25 | J/mol×K | 332.70 | Joback Method |
| cpg | 110.28 | J/mol×K | 361.95 | Joback Method |
| cpg | 115.17 | J/mol×K | 391.19 | Joback Method |
| cpg | 119.94 | J/mol×K | 420.44 | Joback Method |
| cpg | 124.56 | J/mol×K | 449.68 | Joback Method |
| cpg | 129.05 | J/mol×K | 478.93 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| 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=C627418&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307i |

Legend

| | |
|-----------------|---|
| 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 |
| ie: | Ionization energy |
| 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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