Carbonic acid, dimethyl ester

Other names: CH3OCOOCH3; Dimethyl carbonate; Dimethyl ester of carbonic acid; Methyl carbonate; Methyl carbonate ((MeO)2CO); UN 1161.

InChI: InChI=1S/C3H6O3/c1-5-3(4)6-2/h1-2H3

InChI Key: IEJIGPNLZYLBP-UHFFFAOYSA-N

Formula: C3H6O3

SMILES: COC(=O)OC

Molecular Weight: 90.08

CAS: 616-38-6

Physical Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Unit</th>
<th>Source</th>
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</thead>
<tbody>
<tr>
<td>PAff</td>
<td>830.20</td>
<td>kJ/mol</td>
<td>NIST Webbook</td>
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<tr>
<td>BasG</td>
<td>799.20</td>
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</tr>
<tr>
<td>$\Delta_G^\circ$</td>
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<td>Joback Method</td>
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<td>$\Delta_H^\circ_{gas}$</td>
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<tr>
<td>$\Delta_{vap}H^\circ$</td>
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<td>IE</td>
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<td>eV</td>
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<td>eV</td>
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<td>$\log P_{oct/wat}$</td>
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<tr>
<td>$P_c$</td>
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<tr>
<td>$T_{boil}$</td>
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<td>$T_{boil}$</td>
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<tr>
<td>Property</td>
<td>Value</td>
<td>Unit</td>
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<td>NIST Webbook</td>
</tr>
<tr>
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<td>557.00 ± 2.00</td>
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<tr>
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<td>m³/kg-mol</td>
<td>Joback Method</td>
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### Temperature Dependent Properties

<table>
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<th>Property</th>
<th>Value</th>
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<th>Temperature (K)</th>
<th>Source</th>
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<tbody>
<tr>
<td>$C_{p,\text{gas}}$</td>
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<td>kJ/mol</td>
<td>368.5</td>
<td>NIST Webbook</td>
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</tbody>
</table>

### Sources

- **NIST Webbook**: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C3H6O3/c1-5-3(4)6-2/h1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C3H6O3/c1-5-3(4)6-2/h1-2H3)

### Legend

- **PAff**: Proton affinity (kJ/mol).
- **BasG**: Gas basicity (kJ/mol).
- $C_{p,\text{gas}}$: Ideal gas heat capacity (J/mol×K).
- $\eta$: Dynamic viscosity (Pa×s).
- $\Delta G^\circ$: Standard Gibbs free energy of formation (kJ/mol).
- $\Delta H^\circ_{\text{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
\( \Delta_{\text{fus}} H^\circ \): Enthalpy of fusion at standard conditions (kJ/mol).
\( \Delta_{\text{fus}} H \): Enthalpy of fusion at a given temperature (kJ/mol).
\( \Delta_{\text{vap}} H^\circ \): Enthalpy of vaporization at standard conditions (kJ/mol).
\( \Delta_{\text{vap}} H \): Enthalpy of vaporization at a given temperature (kJ/mol).
IE: Ionization energy (eV).

\( \log P_{\text{oct/wat}} \): Octanol/Water partition coefficient.
\( P_c \): Critical Pressure (kPa).
\( T_{\text{boil}} \): Normal Boiling Point Temperature (K).
\( T_c \): Critical Temperature (K).
\( T_{\text{fus}} \): Normal melting (fusion) point (K).
\( V_c \): Critical Volume (m\(^3\)/kg-mol).

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