

# Ether, sec-butyl isopropyl

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Sec-butyl isopropyl ether                        |
| <b>Inchi:</b>               | InChI=1S/C7H16O/c1-5-7(4)8-6(2)3/h6-7H,5H2,1-4H3 |
| <b>InchiKey:</b>            | QHJLNXCCHSKDYHR-UHFFFAOYSA-N                     |
| <b>Formula:</b>             | C7H16O   |
| <b>SMILES:</b>              | CCC(C)OC(C)C                                     |
| <b>Mol. weight [g/mol]:</b> | 116.20   |
| <b>CAS:</b>                 | 18641-81-1                                       |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -101.82 | kJ/mol               | Joback Method  |
| hf            | -330.59 | kJ/mol               | Joback Method  |
| hfus          | 8.03    | kJ/mol               | Joback Method  |
| hvap          | 37.58   | kJ/mol               | NIST Webbook   |
| log10ws       | -2.06   |                      | Crippen Method |
| logp          | 2.210   |                      | Crippen Method |
| mcvol         | 115.360 | ml/mol               | McGowan Method |
| pc            | 2796.51 | kPa                  | Joback Method  |
| tb            | 373.20  | K                    | NIST Webbook   |
| tc            | 553.18  | K                    | Joback Method  |
| tf            | 160.88  | K                    | Joback Method  |
| vc            | 0.433   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 285.76    | J/molxK | 553.18          | Joback Method |
| cpg           | 218.23    | J/molxK | 381.10          | Joback Method |
| cpg           | 230.43    | J/molxK | 409.78          | Joback Method |
| cpg           | 242.25    | J/molxK | 438.46          | Joback Method |
| cpg           | 253.69    | J/molxK | 467.14          | Joback Method |
| cpg           | 264.76    | J/molxK | 495.82          | Joback Method |
| cpg           | 275.45    | J/molxK | 524.50          | Joback Method |
| dvisc         | 0.0002095 | Paxs    | 381.10          | Joback Method |

|       |           |        |        |               |
|-------|-----------|--------|--------|---------------|
| dvisc | 0.0138704 | Paxs   | 160.88 | Joback Method |
| dvisc | 0.0036036 | Paxs   | 197.58 | Joback Method |
| dvisc | 0.0014282 | Paxs   | 234.29 | Joback Method |
| dvisc | 0.0007273 | Paxs   | 270.99 | Joback Method |
| dvisc | 0.0004351 | Paxs   | 307.69 | Joback Method |
| dvisc | 0.0002904 | Paxs   | 344.40 | Joback Method |
| hvapt | 32.38     | kJ/mol | 373.20 | NIST Webbook  |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>   |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C18641811&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18641811&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                     |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>hvapt:</b>   | Enthalpy of vaporization at a given temperature |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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