

# Isopropyl acrylate

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 1-methylethyl 2-propenoate<br>2-Propenoic acid, 1-methylethyl ester<br>2-Propenoic acid,isopropyl ester<br>Acrylic acid, isopropyl ester<br>Isopropyl 2-propenoate<br>Isopropyl ester of 2-propenoic acid |
| <b>Inchi:</b>               | InChI=1S/C6H10O2/c1-4-6(7)8-5(2)3/h4-5H,1H2,2-3H3   |
| <b>InchiKey:</b>            | LYBIZMNPXTXVMV-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C6H10O2   |
| <b>SMILES:</b>              | C=CC(=O)OC(C)C  |
| <b>Mol. weight [g/mol]:</b> | 114.14  |
| <b>CAS:</b>                 | 689-12-3  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -148.88 | kJ/mol               | Joback Method  |
| hf            | -291.82 | kJ/mol               | Joback Method  |
| hfus          | 9.28    | kJ/mol               | Joback Method  |
| hvap          | 37.05   | kJ/mol               | Joback Method  |
| log10ws       | -1.16   |                      | Crippen Method |
| logp          | 1.124   |                      | Crippen Method |
| mcvol         | 98.540  | ml/mol               | McGowan Method |
| pc            | 3468.36 | kPa                  | Joback Method  |
| rinpola       | 722.00  |                      | NIST Webbook   |
| ripola        | 996.00  |                      | NIST Webbook   |
| tb            | 409.21  | K                    | Joback Method  |
| tc            | 594.78  | K                    | Joback Method  |
| tf            | 212.78  | K                    | Joback Method  |
| vc            | 0.370   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 184.94 | J/mol×K | 409.21          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 194.42    | J/molxK | 440.14 | Joback Method |
| cpg   | 203.56    | J/molxK | 471.07 | Joback Method |
| cpg   | 212.35    | J/molxK | 502.00 | Joback Method |
| cpg   | 220.81    | J/molxK | 532.93 | Joback Method |
| cpg   | 228.92    | J/molxK | 563.86 | Joback Method |
| cpg   | 236.69    | J/molxK | 594.78 | Joback Method |
| dvisc | 0.0040214 | Paxs    | 212.78 | Joback Method |
| dvisc | 0.0018765 | Paxs    | 245.52 | Joback Method |
| dvisc | 0.0010476 | Paxs    | 278.26 | Joback Method |
| dvisc | 0.0006612 | Paxs    | 311.00 | Joback Method |
| dvisc | 0.0004556 | Paxs    | 343.73 | Joback Method |
| dvisc | 0.0003349 | Paxs    | 376.47 | Joback Method |
| dvisc | 0.0002586 | Paxs    | 409.21 | Joback Method |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.36320e+01                   |
| Coeff. B                    | -3.14702e+03                  |
| Coeff. C                    | -4.76660e+01                  |
| Temperature range (K), min. | 283.50                        |
| Temperature range (K), max. | 425.89                        |

## Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Phase behavior measurement on the binary mixture for isopropyl acrylate and methyl methacrylate in

<https://www.doi.org/10.1016/j.fluid.2006.08.019>

supercritical CO<sub>2</sub>:

[https://en.wikipedia.org/wiki/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=C689123&Units=SI>

The Yaws Handbook of Vapor Pressure:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

# 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>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>pvap:</b>     | Vapor pressure                                  |
| <b>rinpolar:</b> | Non-polar retention indices                     |
| <b>ripolar:</b>  | Polar retention indices                         |
| <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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