

# Acetic acid, iodo-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Iodoacetic acid<br>Monoiodoacetic acid<br>MIA<br>CH <sub>2</sub> ICOOH<br>IA<br>Kyselina jodoctova |
| <b>Inchi:</b>               | InChI=1S/C2H3IO2/c3-1-2(4)5/h1H2,(H,4,5)   |
| <b>InchiKey:</b>            | JDNTWHVOXJZDSN-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C <sub>2</sub> H <sub>3</sub> IO <sub>2</sub>  |
| <b>SMILES:</b>              | O=C(O)CI   |
| <b>Mol. weight [g/mol]:</b> | 185.95   |
| <b>CAS:</b>                 | 64-69-7  |

## Physical Properties

| Property code | Value        | Unit                 | Source         |
|---------------|--------------|----------------------|----------------|
| gf            | -241.66      | kJ/mol               | Joback Method  |
| hf            | -272.55      | kJ/mol               | Joback Method  |
| hfus          | 11.03        | kJ/mol               | Joback Method  |
| hsub          | 86.50 ± 1.00 | kJ/mol               | NIST Webbook   |
| hvap          | 52.84        | kJ/mol               | Joback Method  |
| ie            | 9.60         | eV                   | NIST Webbook   |
| ie            | 11.03        | eV                   | NIST Webbook   |
| log10ws       | -0.71        |                      | Crippen Method |
| logp          | 0.506        |                      | Crippen Method |
| mcvol         | 72.300       | ml/mol               | McGowan Method |
| pc            | 6132.23      | kPa                  | Joback Method  |
| tb            | 484.35       | K                    | Joback Method  |
| tc            | 693.92       | K                    | Joback Method  |
| tf            | 281.11       | K                    | Joback Method  |
| vc            | 0.261        | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

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

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 105.34    | J/mol×K | 484.35 | Joback Method |
| cpg   | 108.85    | J/mol×K | 519.28 | Joback Method |
| cpg   | 112.12    | J/mol×K | 554.21 | Joback Method |
| cpg   | 115.17    | J/mol×K | 589.14 | Joback Method |
| cpg   | 118.02    | J/mol×K | 624.07 | Joback Method |
| cpg   | 120.68    | J/mol×K | 658.99 | Joback Method |
| cpg   | 123.16    | J/mol×K | 693.92 | Joback Method |
| dvisc | 0.0229367 | Paxs    | 281.11 | Joback Method |
| dvisc | 0.0077986 | Paxs    | 314.98 | Joback Method |
| dvisc | 0.0032696 | Paxs    | 348.86 | Joback Method |
| dvisc | 0.0015988 | Paxs    | 382.73 | Joback Method |
| dvisc | 0.0008782 | Paxs    | 416.60 | Joback Method |
| dvisc | 0.0005279 | Paxs    | 450.48 | Joback Method |
| dvisc | 0.0003407 | Paxs    | 484.35 | Joback Method |
| hfust | 15.50     | kJ/mol  | 355.10 | 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=C64697&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C64697&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>hfust:</b>   | Enthalpy of fusion at a given temperature       |
| <b>hsub:</b>    | Enthalpy of sublimation at standard conditions  |
| <b>hvp:</b>     | Enthalpy of vaporization at standard conditions |
| <b>ie:</b>      | Ionization energy                               |
| <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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