

# ethyl succinic acid

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 2-Ethylbutanedioic acid  |
| <b>Inchi:</b>               | InChI=1S/C6H10O4/c1-2-4(6(9)10)3-5(7)8/h4H,2-3H2,1H3,(H,7,8)(H,9,10) |
| <b>InchiKey:</b>            | RVHOBHMAPRVOLO-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C6H10O4  |
| <b>SMILES:</b>              | CCC(CC(=O)O)C(=O)O   |
| <b>Mol. weight [g/mol]:</b> | 146.14   |
| <b>CAS:</b>                 | 636-48-6   |

## Physical Properties

| Property code | Value           | Unit                 | Source         |
|---------------|-----------------|----------------------|----------------|
| chs           | -2801.00 ± 1.40 | kJ/mol               | NIST Webbook   |
| gf            | -534.28         | kJ/mol               | Joback Method  |
| hf            | -702.07         | kJ/mol               | Joback Method  |
| hfus          | 19.15           | kJ/mol               | Joback Method  |
| hvap          | 75.41           | kJ/mol               | Joback Method  |
| log10ws       | -0.29           |                      | Crippen Method |
| logp          | 0.572           |                      | Crippen Method |
| mcvol         | 110.280         | ml/mol               | McGowan Method |
| pc            | 4590.15         | kPa                  | Joback Method  |
| tb            | 628.34          | K                    | Joback Method  |
| tc            | 804.84          | K                    | Joback Method  |
| tf            | 363.88          | K                    | Joback Method  |
| vc            | 0.415           | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 278.07 | J/mol×K | 628.34          | Joback Method |
| cpg           | 285.25 | J/mol×K | 657.76          | Joback Method |
| cpg           | 292.08 | J/mol×K | 687.17          | Joback Method |
| cpg           | 298.55 | J/mol×K | 716.59          | Joback Method |
| cpg           | 304.69 | J/mol×K | 746.00          | Joback Method |
| cpg           | 310.49 | J/mol×K | 775.42          | Joback Method |
| cpg           | 315.96 | J/mol×K | 804.84          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0095884 | Paxs | 363.88 | Joback Method |
| dvisc | 0.0022752 | Paxs | 407.96 | Joback Method |
| dvisc | 0.0007147 | Paxs | 452.03 | Joback Method |
| dvisc | 0.0002758 | Paxs | 496.11 | Joback Method |
| dvisc | 0.0001243 | Paxs | 540.19 | Joback Method |
| dvisc | 0.0000632 | Paxs | 584.26 | Joback Method |
| dvisc | 0.0000353 | Paxs | 628.34 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C636486&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C636486&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>                                 |
| <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>                     |

## Legend

|                 |   |
|-----------------|---|
| <b>chs:</b>     | Standard solid enthalpy of combustion           |
| <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>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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