

# 2-Butenedioic acid, 2-methyl-, (Z)-

|                      |                                                                                                                                                   |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Citraconic acid<br>Methylmaleic acid<br>cis-Methylbutenedioic acid<br>Maleic acid, methyl-<br>Kyselina citrakonova<br>2-Methyl-2-butenedioic acid |
| Inchi:               | InChI=1S/C5H6O4/c1-3(5(8)9)2-4(6)7/h2H,1H3,(H,6,7)(H,8,9)/b3-2-                                                                                   |
| InchiKey:            | HNEGQIOMVPPMNR-IHWYPQMZSA-N                                                                                                                       |
| Formula:             | C5H6O4                                                                                                                                            |
| SMILES:              | CC(=CC(=O)O)C(=O)O                                                                                                                                |
| Mol. weight [g/mol]: | 130.10                                                                                                                                            |
| CAS:                 | 498-23-7                                                                                                                                          |

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| gf            | -468.59       | kJ/mol  | Joback Method  |
| hf            | -568.72       | kJ/mol  | Joback Method  |
| hfus          | 18.97         | kJ/mol  | Joback Method  |
| hvap          | 73.61         | kJ/mol  | Joback Method  |
| log10ws       | 0.03          |         | Crippen Method |
| logp          | 0.102         |         | Crippen Method |
| mcvol         | 91.890        | ml/mol  | McGowan Method |
| pc            | 5644.74       | kPa     | Joback Method  |
| rinpol        | 1222.00       |         | NIST Webbook   |
| tb            | 609.94        | K       | Joback Method  |
| tc            | 793.59        | K       | Joback Method  |
| tf            | 356.40 ± 0.60 | K       | NIST Webbook   |
| tf            | 356.15 ± 0.70 | K       | NIST Webbook   |
| vc            | 0.346         | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 210.67 | J/mol×K | 609.94          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 216.17 | J/mol×K | 640.55 | Joback Method |
| cpg | 221.35 | J/mol×K | 671.16 | Joback Method |
| cpg | 226.24 | J/mol×K | 701.77 | Joback Method |
| cpg | 230.85 | J/mol×K | 732.37 | Joback Method |
| cpg | 235.19 | J/mol×K | 762.98 | Joback Method |
| cpg | 239.29 | J/mol×K | 793.59 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=C498237&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C498237&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>                                     |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <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>rinpola:</b> | Non-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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