

# 2-Butenal

|                      |                                     |
|----------------------|-------------------------------------|
| Other names:         | 1-Formylpropene                     |
|                      | 2-Butenaldehyde                     |
|                      | BETA-METHYLACROLEIN                 |
|                      | But-2-enal                          |
|                      | Crotonal                            |
|                      | Crotonaldehyde                      |
|                      | Crotonic aldehyde                   |
|                      | Crotylaldehyde                      |
|                      | Krotonaldehyd                       |
|                      | NSC 56354                           |
|                      | Propylene aldehyde                  |
|                      | Rcra waste number U053              |
|                      | TRANS-2-BUTENAL                     |
|                      | UN 1143                             |
|                      | «beta»-Methylacrolein               |
|                      | Â«betaÂ»-Methylacrolein             |
| Inchi:               | InChI=1S/C4H6O/c1-2-3-4-5/h2-4H,1H3 |
| InchiKey:            | MLUCVPSAIODCQM-UHFFFAOYSA-N         |
| Formula:             | C4H6O                               |
| SMILES:              | CC=CC=O                             |
| Mol. weight [g/mol]: | 70.09                               |
| CAS:                 | 4170-30-3                           |

## Physical Properties

| Property code | Value           | Unit   | Source        |
|---------------|-----------------|--------|---------------|
| affp          | 830.80          | kJ/mol | NIST Webbook  |
| basg          | 799.00          | kJ/mol | NIST Webbook  |
| chl           | -2284.70 ± 2.30 | kJ/mol | NIST Webbook  |
| chl           | -2287.40 ± 0.40 | kJ/mol | NIST Webbook  |
| gf            | -36.50          | kJ/mol | Joback Method |
| hf            | -100.50 ± 1.50  | kJ/mol | NIST Webbook  |
| hf            | -106.90         | kJ/mol | NIST Webbook  |
| hf            | -109.70 ± 2.40  | kJ/mol | NIST Webbook  |
| hfl           | -138.60 ± 1.90  | kJ/mol | NIST Webbook  |
| hfl           | -144.10 ± 0.40  | kJ/mol | NIST Webbook  |
| hfl           | -146.90 ± 2.40  | kJ/mol | NIST Webbook  |
| hfus          | 8.61            | kJ/mol | Joback Method |

|         |                |        |                                      |
|---------|----------------|--------|--------------------------------------|
| hvap    | 37.30 ± 0.40   | kJ/mol | NIST Webbook                         |
| hvap    | 37.30 ± 0.40   | kJ/mol | NIST Webbook                         |
| hvap    | 37.20          | kJ/mol | NIST Webbook                         |
| hvap    | 38.10          | kJ/mol | NIST Webbook                         |
| hvap    | 38.00 ± 0.80   | kJ/mol | NIST Webbook                         |
| ie      | 9.73 ± 0.01    | eV     | NIST Webbook                         |
| ie      | 9.75           | eV     | NIST Webbook                         |
| ie      | 9.86 ± 0.03    | eV     | NIST Webbook                         |
| log10ws | 0.32           |        | Aqueous Solubility Prediction Method |
| log10ws | 0.32           |        | Estimated Solubility Method          |
| logp    | 0.761          |        | Crippen Method                       |
| mccvol  | 64.490         | ml/mol | McGowan Method                       |
| nfpaf   | %!d(float64=3) |        | KDB                                  |
| nfpah   | %!d(float64=3) |        | KDB                                  |
| nfpas   | %!d(float64=2) |        | KDB                                  |
| pc      | 5496.90 ± 1.00 | kPa    | NIST Webbook                         |
| rhoc    | 293.00 ± 2.80  | kg/m3  | NIST Webbook                         |
| rinpol  | 600.00         |        | NIST Webbook                         |
| rinpol  | 640.00         |        | NIST Webbook                         |
| rinpol  | 627.00         |        | NIST Webbook                         |
| rinpol  | 640.00         |        | NIST Webbook                         |
| rinpol  | 622.00         |        | NIST Webbook                         |
| rinpol  | 655.00         |        | NIST Webbook                         |
| rinpol  | 627.00         |        | NIST Webbook                         |
| rinpol  | 629.00         |        | NIST Webbook                         |
| rinpol  | 648.00         |        | NIST Webbook                         |
| rinpol  | 623.00         |        | NIST Webbook                         |
| rinpol  | 640.00         |        | NIST Webbook                         |
| rinpol  | 627.00         |        | NIST Webbook                         |
| rinpol  | 657.00         |        | NIST Webbook                         |
| rinpol  | 657.00         |        | NIST Webbook                         |
| rinpol  | 618.00         |        | NIST Webbook                         |
| rinpol  | 645.00         |        | NIST Webbook                         |
| rinpol  | 632.00         |        | NIST Webbook                         |
| rinpol  | 630.00         |        | NIST Webbook                         |
| rinpol  | 647.00         |        | NIST Webbook                         |
| rinpol  | 630.00         |        | NIST Webbook                         |
| rinpol  | 619.00         |        | NIST Webbook                         |
| rinpol  | 631.00         |        | NIST Webbook                         |
| rinpol  | 621.00         |        | NIST Webbook                         |
| rinpol  | 615.00         |        | NIST Webbook                         |
| rinpol  | 626.00         |        | NIST Webbook                         |
| rinpol  | 624.00         |        | NIST Webbook                         |

|        |               |         |                                         |
|--------|---------------|---------|-----------------------------------------|
| rinpol | 636.00        |         | NIST Webbook                            |
| rinpol | 621.00        |         | NIST Webbook                            |
| rinpol | 623.00        |         | NIST Webbook                            |
| rinpol | 610.00        |         | NIST Webbook                            |
| ripol  | 1086.20       |         | NIST Webbook                            |
| ripol  | 1086.20       |         | NIST Webbook                            |
| ripol  | 1041.00       |         | NIST Webbook                            |
| ripol  | 1038.00       |         | NIST Webbook                            |
| ripol  | 1056.00       |         | NIST Webbook                            |
| ripol  | 1051.00       |         | NIST Webbook                            |
| ripol  | 1038.00       |         | NIST Webbook                            |
| ripol  | 1047.00       |         | NIST Webbook                            |
| ripol  | 1042.00       |         | NIST Webbook                            |
| ripol  | 1049.00       |         | NIST Webbook                            |
| ripol  | 1056.00       |         | NIST Webbook                            |
| ripol  | 1043.00       |         | NIST Webbook                            |
| ripol  | 1041.00       |         | NIST Webbook                            |
| ripol  | 1024.00       |         | NIST Webbook                            |
| ripol  | 1050.00       |         | NIST Webbook                            |
| ripol  | 1042.00       |         | NIST Webbook                            |
| ripol  | 1042.00       |         | NIST Webbook                            |
| ripol  | 1051.00       |         | NIST Webbook                            |
| ripol  | 1059.00       |         | NIST Webbook                            |
| ripol  | 1069.30       |         | NIST Webbook                            |
| ripol  | 1061.50       |         | NIST Webbook                            |
| ripol  | 1042.00       |         | NIST Webbook                            |
| ripol  | 1077.10       |         | NIST Webbook                            |
| tb     | 375.30 ± 1.50 | K       | NIST Webbook                            |
| tb     | 377.20 ± 0.30 | K       | NIST Webbook                            |
| tb     | 363.15 ± 5.00 | K       | NIST Webbook                            |
| tb     | 375.50 ± 0.60 | K       | NIST Webbook                            |
| tb     | 375.50 ± 0.02 | K       | NIST Webbook                            |
| tc     | 601.98 ± 0.10 | K       | NIST Webbook                            |
| tf     | 196.95        | K       | Aqueous Solubility<br>Prediction Method |
| tf     | 198.00 ± 5.00 | K       | NIST Webbook                            |
| tf     | 196.70 ± 0.50 | K       | NIST Webbook                            |
| tf     | 199.15 ± 1.50 | K       | NIST Webbook                            |
| vc     | 0.257         | m3/kmol | Joback Method                           |

## Temperature Dependent Properties

| Property code | Value        | Unit    | Temperature [K] | Source        |
|---------------|--------------|---------|-----------------|---------------|
| cpg           | 127.50       | J/mol×K | 495.94          | Joback Method |
| cpg           | 110.66       | J/mol×K | 404.62          | Joback Method |
| cpg           | 104.42       | J/mol×K | 374.18          | Joback Method |
| cpg           | 97.86        | J/mol×K | 343.74          | Joback Method |
| cpg           | 116.57       | J/mol×K | 435.06          | Joback Method |
| cpg           | 132.55       | J/mol×K | 526.38          | Joback Method |
| cpg           | 122.18       | J/mol×K | 465.50          | Joback Method |
| dvisc         | 0.0027814    | Pa×s    | 171.76          | Joback Method |
| dvisc         | 0.0002298    | Pa×s    | 343.74          | Joback Method |
| dvisc         | 0.0002883    | Pa×s    | 315.08          | Joback Method |
| dvisc         | 0.0003783    | Pa×s    | 286.41          | Joback Method |
| dvisc         | 0.0005275    | Pa×s    | 257.75          | Joback Method |
| dvisc         | 0.0007992    | Pa×s    | 229.09          | Joback Method |
| dvisc         | 0.0013638    | Pa×s    | 200.42          | Joback Method |
| hvapt         | 37.30        | kJ/mol  | 340.50          | NIST Webbook  |
| hvapt         | 35.10 ± 0.50 | kJ/mol  | 332.00          | NIST Webbook  |
| hvapt         | 38.80        | kJ/mol  | 325.00          | NIST Webbook  |
| hvapt         | 36.80        | kJ/mol  | 341.00          | NIST Webbook  |

## Sources

|                                              |                                                                                                                                                                                                                         |
|----------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>KDB:</b>                                  | <a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1252">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1252</a>                                                                     |
| <b>Aqueous Solubility Prediction Method:</b> | <a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx</a> |
| <b>Estimated Solubility Method:</b>          | <a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</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=C4170303&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4170303&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>Joback Method:</b>                        | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                                                                                                   |

## Legend

|               |                                         |
|---------------|-----------------------------------------|
| <b>affp:</b>  | Proton affinity                         |
| <b>basg:</b>  | Gas basicity                            |
| <b>chl:</b>   | Standard liquid 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>hfl:</b>     | Liquid phase 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>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>nfpaf:</b>   | NFPA Fire Rating                                          |
| <b>nfpah:</b>   | NFPA Health Rating                                        |
| <b>nfpas:</b>   | NFPA Safety Rating                                        |
| <b>pc:</b>      | Critical Pressure                                         |
| <b>rhoc:</b>    | Critical density                                          |
| <b>rinpol:</b>  | Non-polar retention indices                               |
| <b>ripol:</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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