

# CH<sub>2</sub>=C

|                      |                             |
|----------------------|-----------------------------|
| Inchi:               | InChI=1S/C2H2/c1-2/h1H2     |
| InchiKey:            | SNVLJLYUUXKWOJ-UHFFFAOYSA-N |
| Formula:             | C2H2                        |
| SMILES:              | [C]=C                       |
| Mol. weight [g/mol]: | 26.04                       |
| CAS:                 | 2143-69-3                   |

## Physical Properties

| Property code | Value       | Unit   | Source         |
|---------------|-------------|--------|----------------|
| ea            | 0.43        | eV     | NIST Webbook   |
| ea            | 0.48 ± 0.01 | eV     | NIST Webbook   |
| ea            | 0.45 ± 0.00 | eV     | NIST Webbook   |
| ea            | 0.48 ± 0.21 | eV     | NIST Webbook   |
| ea            | 0.49 ± 0.01 | eV     | NIST Webbook   |
| ea            | 0.47 ± 0.02 | eV     | NIST Webbook   |
| log10ws       | -0.09       |        | Crippen Method |
| logp          | 0.482       |        | Crippen Method |
| mcvol         | 30.440      | ml/mol | McGowan Method |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2143693&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2143693&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                   |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |

## Legend

|          |                                     |
|----------|-------------------------------------|
| ea:      | Electron affinity                   |
| log10ws: | Log10 of Water solubility in mol/l  |
| logp:    | Octanol/Water partition coefficient |

**mcvol:** McGowan's characteristic volume

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