

# 5-HEXENAL, 4-METHYLENE-

|                      |                                                  |
|----------------------|--------------------------------------------------|
| Other names:         | 4-Methylidenehex-5-enal                          |
| Inchi:               | InChI=1S/C7H10O/c1-3-7(2)5-4-6-8/h3,6H,1-2,4-5H2 |
| InchiKey:            | GTQGBVLUEUNXCG-UHFFFAOYSA-N                      |
| Formula:             | C7H10O                                           |
| SMILES:              | C=CC(=C)CCC=O                                    |
| Mol. weight [g/mol]: | 110.16                                           |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hfus          | 12.30   | kJ/mol | Joback Method      |
| hvap          | 46.12   | kJ/mol | Cheméo Relay (1.0) |
| logp          | 1.708   |        | Crippen Method     |
| mcvol         | 102.460 | ml/mol | McGowan Method     |
| rinpol        | 896.80  |        | NIST Webbook       |
| rinpol        | 896.80  |        | NIST Webbook       |
| tb            | 411.09  | K      | Cheméo Relay (1.0) |
| tf            | 212.82  | K      | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 187.15 | J/mol×K | 401.46          | Joback Method |
| cpg           | 197.09 | J/mol×K | 431.87          | Joback Method |
| cpg           | 206.56 | J/mol×K | 462.29          | Joback Method |
| cpg           | 215.56 | J/mol×K | 492.70          | Joback Method |
| cpg           | 224.12 | J/mol×K | 523.12          | Joback Method |
| cpg           | 232.25 | J/mol×K | 553.53          | Joback Method |
| cpg           | 239.97 | J/mol×K | 583.95          | Joback Method |

## Sources

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C17844212&Units=SI>

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

|                |                                                 |
|----------------|-------------------------------------------------|
| <b>cpg:</b>    | Ideal gas heat capacity                         |
| <b>hfus:</b>   | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>   | Enthalpy of vaporization at standard conditions |
| <b>logp:</b>   | Octanol/Water partition coefficient             |
| <b>mcvol:</b>  | McGowan's characteristic volume                 |
| <b>rinpol:</b> | Non-polar retention indices                     |
| <b>tb:</b>     | Normal Boiling Point Temperature                |
| <b>tf:</b>     | Normal melting (fusion) point                   |

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