

# Bicyclo[2.2.2]oct-2-ene, 5-ethyl-, (1«alpha»,4«alpha»,5«alpha»)-

**Inchi:** InChI=1S/C10H16/c1-2-9-7-8-3-5-10(9)6-4-8/h3,5,8-10H,2,4,6-7H2,1H3/t8?,9-,10-/m1/s1

**InchiKey:** FTOFVYGLRHSFAM-HWOCKDDLSA-N

**Formula:** C10H16

**SMILES:** CCC1CC2C=CC1CC2

**Mol. weight [g/mol]:** 136.23

**CAS:** 106623-86-3

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| gf            | 152.87        | kJ/mol  | Joback Method  |
| hf            | -30.00 ± 4.20 | kJ/mol  | NIST Webbook   |
| hfus          | 16.02         | kJ/mol  | Joback Method  |
| hvap          | 38.01         | kJ/mol  | Joback Method  |
| log10ws       | -2.93         |         | Crippen Method |
| logp          | 2.999         |         | Crippen Method |
| mcvol         | 125.740       | ml/mol  | McGowan Method |
| pc            | 2875.03       | kPa     | Joback Method  |
| tb            | 444.71        | K       | Joback Method  |
| tc            | 651.61        | K       | Joback Method  |
| tf            | 227.82        | K       | Joback Method  |
| vc            | 0.478         | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 271.38    | J/mol×K | 444.71          | Joback Method |
| cpg           | 290.61    | J/mol×K | 479.19          | Joback Method |
| cpg           | 308.70    | J/mol×K | 513.68          | Joback Method |
| cpg           | 325.70    | J/mol×K | 548.16          | Joback Method |
| cpg           | 341.67    | J/mol×K | 582.64          | Joback Method |
| cpg           | 356.67    | J/mol×K | 617.12          | Joback Method |
| cpg           | 370.74    | J/mol×K | 651.61          | Joback Method |
| dvisc         | 0.0009901 | Pa×s    | 227.82          | Joback Method |
| dvisc         | 0.0008249 | Pa×s    | 263.97          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0007182 | Pa×s | 300.12 | Joback Method |
| dvisc | 0.0006441 | Pa×s | 336.26 | Joback Method |
| dvisc | 0.0005901 | Pa×s | 372.41 | Joback Method |
| dvisc | 0.0005490 | Pa×s | 408.56 | Joback Method |
| dvisc | 0.0005168 | Pa×s | 444.71 | Joback Method |

## Sources

|                        |                                                                                                                                                 |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                           |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C106623863&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C106623863&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>                               |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <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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