

# Bicyclo[3.3.0]octa-2,7-diene

|                      |                                                       |
|----------------------|-------------------------------------------------------|
| Inchi:               | InChI=1S/C8H10/c1-3-7-5-2-6-8(7)4-1/h1-3,5,7-8H,4,6H2 |
| InchiKey:            | KWMNZJNIAZZNSJ-UHFFFAOYSA-N                           |
| Formula:             | C8H10                                                 |
| SMILES:              | C1=CC2C=CCC2C1                                        |
| Mol. weight [g/mol]: | 106.17                                                |
| CAS:                 | 41164-14-1                                            |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 173.70  | kJ/mol  | Joback Method  |
| hf            | 40.39   | kJ/mol  | Joback Method  |
| hfus          | 10.99   | kJ/mol  | Joback Method  |
| hvap          | 34.16   | kJ/mol  | Joback Method  |
| log10ws       | -2.18   |         | Crippen Method |
| logp          | 2.139   |         | Crippen Method |
| mcvol         | 93.260  | ml/mol  | McGowan Method |
| pc            | 3886.79 | kPa     | Joback Method  |
| tb            | 402.78  | K       | Joback Method  |
| tc            | 617.25  | K       | Joback Method  |
| tf            | 210.28  | K       | Joback Method  |
| vc            | 0.353   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 172.91    | J/mol×K | 402.78          | Joback Method |
| cpg           | 188.64    | J/mol×K | 438.53          | Joback Method |
| cpg           | 203.27    | J/mol×K | 474.27          | Joback Method |
| cpg           | 216.87    | J/mol×K | 510.02          | Joback Method |
| cpg           | 229.50    | J/mol×K | 545.76          | Joback Method |
| cpg           | 241.22    | J/mol×K | 581.51          | Joback Method |
| cpg           | 252.10    | J/mol×K | 617.25          | Joback Method |
| dvisc         | 0.0007709 | Pa×s    | 210.28          | Joback Method |
| dvisc         | 0.0006515 | Pa×s    | 242.36          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0005727 | Pa×s | 274.45 | Joback Method |
| dvisc | 0.0005172 | Pa×s | 306.53 | Joback Method |
| dvisc | 0.0004762 | Pa×s | 338.61 | Joback Method |
| dvisc | 0.0004447 | Pa×s | 370.70 | Joback Method |
| dvisc | 0.0004199 | Pa×s | 402.78 | Joback Method |

## Sources

|                        |                                                                                                                                               |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                                         |
| <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=C41164141&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C41164141&amp;Units=SI</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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