

# trans-Bicyclo[4.1.0]hept-3-ene

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C7H10/c1-2-4-7-5-6(7)3-1/h1-2,6-7H,3-5H2/t6-,7-/m0/s1 |
| InchiKey:            | JBFDZEJAJZJORO-BQBZGAKWSA-N                                    |
| Formula:             | C7H10  |
| SMILES:              | C1=CCC2CC2C1   |
| Mol. weight [g/mol]: | 94.15  |
| CAS:                 | 84194-54-7   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 147.42  | kJ/mol               | Joback Method  |
| hf            | 232.00  | kJ/mol               | NIST Webbook   |
| hfus          | 9.28    | kJ/mol               | Joback Method  |
| hvap          | 31.47   | kJ/mol               | Joback Method  |
| log10ws       | -1.91   |                      | Crippen Method |
| logp          | 1.973   |                      | Crippen Method |
| mcvol         | 83.470  | ml/mol               | McGowan Method |
| pc            | 4062.13 | kPa                  | Joback Method  |
| tb            | 376.47  | K                    | Joback Method  |
| tc            | 581.59  | K                    | Joback Method  |
| tf            | 201.77  | K                    | Joback Method  |
| vc            | 0.320   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 147.84    | J/molxK | 376.47          | Joback Method |
| cpg           | 162.81    | J/molxK | 410.66          | Joback Method |
| cpg           | 176.76    | J/molxK | 444.84          | Joback Method |
| cpg           | 189.74    | J/molxK | 479.03          | Joback Method |
| cpg           | 201.82    | J/molxK | 513.22          | Joback Method |
| cpg           | 213.06    | J/molxK | 547.41          | Joback Method |
| cpg           | 223.52    | J/molxK | 581.59          | Joback Method |
| dvisc         | 0.0004629 | Paxs    | 201.77          | Joback Method |
| dvisc         | 0.0004471 | Paxs    | 230.89          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0004352 | Paxs | 260.00 | Joback Method |
| dvisc | 0.0004260 | Paxs | 289.12 | Joback Method |
| dvisc | 0.0004186 | Paxs | 318.24 | Joback Method |
| dvisc | 0.0004125 | Paxs | 347.35 | Joback Method |
| dvisc | 0.0004074 | Paxs | 376.47 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=C84194547&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C84194547&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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