

# (5R)-5-Hydroxymethylbicyclo[2.2.1]hept-2-ene

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C8H12O/c9-5-8-4-6-1-2-7(8)3-6/h1-2,6-9H,3-5H2/t6?,7?,8-/m0/s1 |
| InchiKey:            | LUMNWCHHXDUKFI-RRQHEKLDSA-N  |
| Formula:             | C8H12O   |
| SMILES:              | OCC1CC2C=CC1C2   |
| Mol. weight [g/mol]: | 124.18   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 11.31   | kJ/mol  | Joback Method  |
| hf            | -183.80 | kJ/mol  | Joback Method  |
| hfus          | 17.03   | kJ/mol  | Joback Method  |
| hvap          | 50.06   | kJ/mol  | Joback Method  |
| log10ws       | -1.35   |         | Crippen Method |
| logp          | 1.191   |         | Crippen Method |
| mcvol         | 103.430 | ml/mol  | McGowan Method |
| pc            | 3877.12 | kPa     | Joback Method  |
| rinpol        | 1050.00 |         | NIST Webbook   |
| tb            | 486.86  | K       | Joback Method  |
| tc            | 679.37  | K       | Joback Method  |
| tf            | 269.62  | K       | Joback Method  |
| vc            | 0.394   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 245.09    | J/molxK | 486.86          | Joback Method |
| cpg           | 258.45    | J/molxK | 518.95          | Joback Method |
| cpg           | 270.99    | J/molxK | 551.03          | Joback Method |
| cpg           | 282.77    | J/molxK | 583.12          | Joback Method |
| cpg           | 293.82    | J/molxK | 615.20          | Joback Method |
| cpg           | 304.20    | J/molxK | 647.29          | Joback Method |
| cpg           | 313.95    | J/molxK | 679.37          | Joback Method |
| dvisc         | 0.0076807 | Paxs    | 269.62          | Joback Method |
| dvisc         | 0.0037686 | Paxs    | 305.83          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0021499 | Paxs | 342.03 | Joback Method |
| dvisc | 0.0013656 | Paxs | 378.24 | Joback Method |
| dvisc | 0.0009390 | Paxs | 414.45 | Joback Method |
| dvisc | 0.0006857 | Paxs | 450.65 | Joback Method |
| dvisc | 0.0005247 | Paxs | 486.86 | 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=R557418&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R557418&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>rinpol:</b>  | Non-polar retention indices                     |
| <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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