

# Hexopyranose

|                      |                                                           |
|----------------------|-----------------------------------------------------------|
| Inchi:               | InChI=1S/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2 |
| InchiKey:            | WQZGKKKJIJFFOK-UHFFFAOYSA-N                               |
| Formula:             | C6H12O6                                                   |
| SMILES:              | OCC1OC(O)C(O)C(O)C1O                                      |
| Mol. weight [g/mol]: | 180.16                                                    |

## Physical Properties

| Property code | Value    | Unit    | Source         |
|---------------|----------|---------|----------------|
| gf            | -776.97  | kJ/mol  | Joback Method  |
| hf            | -1087.36 | kJ/mol  | Joback Method  |
| hfus          | 35.83    | kJ/mol  | Joback Method  |
| hvap          | 116.05   | kJ/mol  | Joback Method  |
| log10ws       | 1.31     |         | Crippen Method |
| logp          | -3.221   |         | Crippen Method |
| mcvol         | 119.760  | ml/mol  | McGowan Method |
| pc            | 6200.01  | kPa     | Joback Method  |
| tb            | 825.40   | K       | Joback Method  |
| tc            | 1011.14  | K       | Joback Method  |
| tf            | 478.47   | K       | Joback Method  |
| vc            | 0.416    | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 418.13    | J/mol×K | 825.40          | Joback Method |
| cpg           | 425.76    | J/mol×K | 856.36          | Joback Method |
| cpg           | 432.81    | J/mol×K | 887.31          | Joback Method |
| cpg           | 439.26    | J/mol×K | 918.27          | Joback Method |
| cpg           | 445.12    | J/mol×K | 949.22          | Joback Method |
| cpg           | 450.39    | J/mol×K | 980.18          | Joback Method |
| cpg           | 455.08    | J/mol×K | 1011.14         | Joback Method |
| dvisc         | 0.0004404 | Pa×s    | 478.47          | Joback Method |
| dvisc         | 0.0000602 | Pa×s    | 536.29          | Joback Method |
| dvisc         | 0.0000121 | Pa×s    | 594.11          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000032 | Pa×s | 651.93 | Joback Method |
| dvisc | 0.0000011 | Pa×s | 709.76 | Joback Method |
| dvisc | 0.0000004 | Pa×s | 767.58 | Joback Method |
| dvisc | 0.0000002 | Pa×s | 825.40 | 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=B6001298&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6001298&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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