

# Lactose

|                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | (+)-Lactose<br>4-(«beta»-D-Galactosido)-D-glucose<br>4-(Â«betaÂ»-D-Galactosido)-D-glucose<br>4-O-.beta.-D-galactopyranosyl-D-glucose<br>AHL<br>Aletobiose<br>D-(+)-lactose<br>D-Glucose, 4-O-«beta»-D-galactopyranosyl-<br>D-Glucose, 4-O-Â«betaÂ»-D-galactopyranosyl-<br>D-Lactose<br>D-glucose, 4-(beta-d-galactosido)-<br>Fast-Flo Lactose<br>Fast-flo<br>Galactinum<br>Lactin<br>Lactin (carbohydrate)<br>Lactobiose<br>Lactose Fast-flo<br>Milk sugar<br>Osmolactan<br>Pharmatose 21<br>Saccharum lacticum<br>Tablettose<br>Zeparox EP |
| Inchi:               | InChI=1S/C12H22O11/c13-1-3-5(15)6(16)9(19)12(22-3)23-10-4(2-14)21-11(20)8(18)7(10)                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| InchiKey:            | GUBGYTABKSRVRQ-SDWOOCBUSA-N                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| Formula:             | C12H22O11                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| SMILES:              | OCC1OC(OC2C(CO)OC(O)C(O)C2O)C(O)C(O)C1O                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| Mol. weight [g/mol]: | 342.30                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| CAS:                 | 63-42-3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |

## Physical Properties

| Property code | Value    | Unit   | Source        |
|---------------|----------|--------|---------------|
| gf            | -1334.42 | kJ/mol | Joback Method |
| hf            | -1959.15 | kJ/mol | Joback Method |
| hfus          | 68.92    | kJ/mol | Joback Method |

|         |         |         |                                      |
|---------|---------|---------|--------------------------------------|
| hvap    | 185.55  | kJ/mol  | Joback Method                        |
| log10ws | -0.24   |         | Aqueous Solubility Prediction Method |
| log10ws | -0.24   |         | Estimated Solubility Method          |
| logp    | -5.397  |         | Crippen Method                       |
| mcvol   | 222.790 | ml/mol  | McGowan Method                       |
| pc      | 4311.22 | kPa     | Joback Method                        |
| tb      | 1289.46 | K       | Joback Method                        |
| tc      | 1783.82 | K       | Joback Method                        |
| tf      | 767.77  | K       | Joback Method                        |
| vc      | 0.777   | m3/kmol | Joback Method                        |

## Temperature Dependent Properties

| Property code | Value         | Unit    | Temperature [K] | Source        |
|---------------|---------------|---------|-----------------|---------------|
| cpg           | 889.71        | J/mol×K | 1289.46         | Joback Method |
| cpg           | 874.12        | J/mol×K | 1371.85         | Joback Method |
| cpg           | 848.56        | J/mol×K | 1454.25         | Joback Method |
| cpg           | 812.80        | J/mol×K | 1536.64         | Joback Method |
| cpg           | 766.60        | J/mol×K | 1619.03         | Joback Method |
| cpg           | 709.75        | J/mol×K | 1701.43         | Joback Method |
| cpg           | 641.99        | J/mol×K | 1783.82         | Joback Method |
| cps           | 417.60        | J/mol×K | 300.00          | NIST Webbook  |
| dvisc         | 2.0238363e-08 | Pa×s    | 767.77          | Joback Method |
| dvisc         | 3.1497617e-09 | Pa×s    | 854.72          | Joback Method |
| dvisc         | 6.9115221e-10 | Pa×s    | 941.67          | Joback Method |
| dvisc         | 1.9598804e-10 | Pa×s    | 1028.62         | Joback Method |
| dvisc         | 6.7640490e-11 | Pa×s    | 1115.56         | Joback Method |
| dvisc         | 2.7226863e-11 | Pa×s    | 1202.51         | Joback Method |
| dvisc         | 1.2390430e-11 | Pa×s    | 1289.46         | Joback Method |

## Sources

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

**Estimated Solubility Method:** [http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C63423&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Volumetric behaviour of amino acids and their group contributions in aqueous solutions  
Effect of fruit and milk sugars on the solubility of different solutes  
Intermolecular interactions of diphenylmethane in aqueous solutions  
Diphenylmethane-hydrochloride drug in aqueous solutions in viewpoint of volumetric and transport properties:

<https://www.doi.org/10.1016/j.jct.2010.08.004>

<https://www.doi.org/10.1016/j.jct.2017.12.013>

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>cps:</b>     | Solid phase 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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