

Biodiesel Package 2021

Data Bank Subset for Biodiesel Related Compounds (DDB Biodiesel)

Yearly 170 Gt of biomass is produced by photosynthesis worldwide. Biomass means mainly fat and oil (predominantly triglycerides), carbohydrates (sugar, starch, cellulose, chitin) and lignin. Today only 3 % of the biomass is used as food, fuel or as construction material, e.g. for furniture, etc.

In particular because of the shortage of oil and gas and the problems caused by CO₂ it seems obvious to use these natural resources as raw material in chemical industry or as energy source.

So for example in chemical industry fat and oil are converted to fatty acids by hydrolysis or fatty acid esters (biodiesel), e.g. FAME manufactured by transesterification. Fatty alcohols can be produced by hydrogenation of fatty acids. For the development of the most economical production process, a reliable knowledge of the thermophysical pure component and mixture properties of the compounds involved is required. These are the different glycerides (tri-, di-, mono glycerides), glycerol, fatty acids, fatty acid alkyl esters, fatty alcohols, the different alcohols used for the transesterification reaction (methanol, ethanol, propanol, butanol, ..).

A great part of the required data are stored in the Dortmund Data Bank (DDB). A detailed description of the Biodiesel Package can be downloaded from www.ddbst.com – Products – Special Applications – Biodiesel Related Data). Besides for biodiesel production and processing, these data are of great value also for other applications like e.g. natural oil extraction and purification.

The amount of biodiesel related data stored in the DDB are given in the table.

Data bank	Sets	Points
Vapor-liquid equilibria	3,800	38,100
Azeotropic data	3,200	3,200
Gas solubilities	620	2,400
Liquid-liquid equilibria	2,300	20,600
Solid-liquid equilibria	3,600	28,800
Activity coefficients at infinite	3,500	3,500
dilution		
Excess enthalpies	890	14,500
Excess heat capacities	100	1,000
Mixture densities	2,400	32,600
Mixture viscosities	2,100	25,300
Electrical conductivities	160	1,300
Octanol-Water partition	110	110
coefficients		
Salt solubilities	230	1,400
Pure component properties	14,400	62,800
Different thermodynamic	4,900	47,200
properties		
Total	42,900	283,800

For the efficient use of these data we would recommend the software package DDBSP. The software package allows retrieving the data using several search options (components, systems, literature), has graphical data representations, has copy and print capabilities, and allows data export to PPDX and Aspen INP files. Furthermore with the help of the software package the user can define new components or store own experimental data. At the same time with the software package the required basic data for the compound used, such as name, formula, CAS registry number, Antoine constants, critical data, acentric factor, density, van der Waals properties, melting point and heat of fusion, dipole moment etc. are delivered.

Changes and errors are possible regarding all information and prices.