DDBST
DORTMUND DATA BANK
SOFTWARE & SEPARATION
TECHNOLOGY

DDBST - Dortmund Data Bank Software & Separation Technology GmbH
Marie-Curie-Str. 10 | D-26129 Oldenburg | Germany

DDB 2018
Biodiesel Package

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 CO_2 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	3,340	32,800
Azeotropic data	3,200	3,200
Gas solubilities	590	2,170
Liquid-liquid equilibria	2,000	18,000
Solid-liquid equilibria	3,100	24,670
Activity coefficients at infinite dilution	3,360	3,360
Excess enthalpies	860	14,000
Excess heat capacities	80	880
Mixture densities	2,100	28,000
Mixture viscosities	1,450	16,380
Electrical conductivities	90	680
Octanol-Water partition coefficients	110	110
Salt solubilities	170	1,170
Pure component properties	12,800	54,760
Different thermodynamic properties	4,360	45,300
...		
Total	**36,650**	**232,180**

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. DDB-Biodiesel including basic parts of DDBSP is available for 11,500 € as an indefinite single PC version. 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.

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Software & Separation Technology GmbH
Marie-Curie-Str. 10 | D-26129 Oldenburg | Germany
P +49-441-361819-0
F +49-441-361819-10
info@ddbst.de | www.ddbst.de

Oldenburgische Landesbank AG
Account No.: 142 6 164 800 | Bank Code: 280 200 50
SWIFT-BIC: OLBO DE H2 | IBAN: DE46 280 200 50 142 6 164 800
HRB Oldenburg 2521 | VAT Reg. No..: DE117 483996

Managing Directors:
Prof. Dr. Jürgen Gmehling,
Dr. Andreas Grybat, Dr. Sven Horstmann,
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