

Dortmund Data Bank (DDB)

Polymer Data Bank

The Polymer Data Bank was developed at DDBST GmbH between 2003 and 2005.

Main Responsibilities:

- Jörg Krafczyk (DDBST GmbH)
 - Data Base Structure
 - Development System Implementation
 - Data Input Supervision
- Prof. Dr. Christian Wohlfarth (Martin Luther University Halle-Wittenberg)
 - Scientific Consulting
 - Literature Sources (PhD-thesis, Industry Reports, ...)
- Wilfried Cordes (DDBST GmbH)
 - Implementation of the Polymer Data Bank into DDBSP
- Johannes Weinert (DDBST GmbH)
 - Implementation of Graphical Representations, ...

**This is the first public presentation of the Data Bank.
Suggestions for improvements are welcome and can still be
implemented without huge effort.**

		Data Sets
VLE Data	Binary	2300
	Ternary	180
LLE Data	Binary	1700
	Ternary	1350
Gas/Vapor/Solvent Solubility Data		7300
PVT Data for Polymers		310
H ^E and H _{dilution} Data for Polymer/Solvent Systems		500
V ^E and Density Data for Polymer/Solvent Systems		680
Other Properties (Swelling, Partition Coefficients, ...)		380
total	133 181 data points, 4937 sets containing only one data point	14700

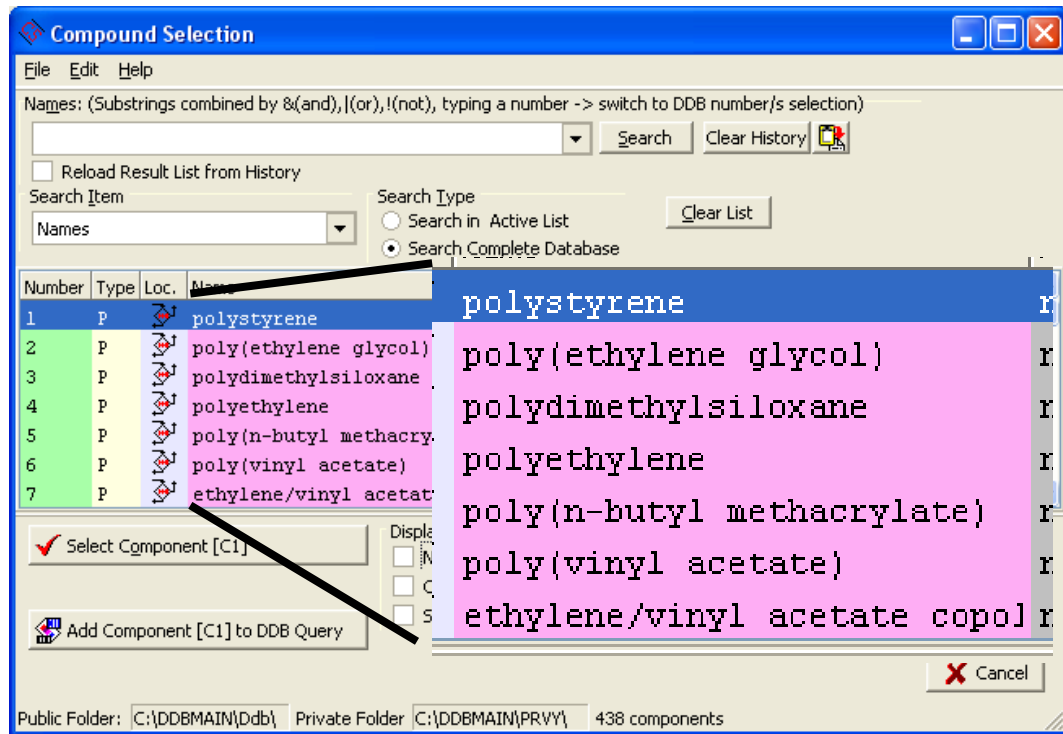
Supporting DDBSP-Software is under Further Development

Current features include basic search, retrieval and plot capabilities and private data input. Integration of correlation and estimation methods is planned for the future.

The Polymer Data Bank is fully integrated into the DDBSP user interface.

- Based on all compilations of C. Wohlfarth original sources were reevaluated with respect to the published properties
- Further input within the usual DDB update procedure
- Reevaluation of other compilations (e.g. Alessi, Kikic) and integration of further properties planned

- Currently 438 Polymers and Co-Polymers
- Further Specifications in each Data Set:



Constants		Polymer/Component Details				Comment	
#Polymer/Comp't	#Index	WMN	WMW	WMZ	WMETA	Additional Information	Additional Information
3000004	1 Polymer B	1710	3710				
27	2 Component A						

PVT		
PVT	volume expansion coeff.	
LLE		
LLE	cloud points	
LLE	cloud points, UCST	
LLE	cloud points, UCST/LCST-merging behavior	
LLE	cloud points, LCST	
LLE	spinodal points	
LLE	coexistence data	
LLE	coexistence data	tie lines
LLE	partition coefficients	eight fraction based, "from to Forma
LLE	partition coefficients	weight fraction based
LLE	spinodal points (LCST)	
LLE	UCST	UCST given
LLE	LCST	LCST given
LLE	cloud points, UCST	UCST given
LLE	cloud points, LCP/UCP branch	
LLE	cloud points, UCP behavior	
LLE	binodal points	
LLE	fract. by demixing	
LLE	spinodal points (UCST)	
LLE	tie lines (UCST)	demixing Temperature given
LLE	tie lines (LCST)	demixing Temperature given
LLE	cloud points, LCST, precipitation threshold	
LLE	cloud points, UCST, precipitation threshold	
LLE	isotropic/nematic LLE, coexistence data	
LLE	binodal data (UCST)	
LLE	plait point composition	

LLE	critical point	
LLE	cloud point, threshold point	
LLE	phase data of isotropic-isotropic and isotropic-nematic equilibrium	
LLE	cloud point (critical point)	
LLE	cloud points (precipitation threshold)	
LLE	cloud points and spinodal points	
LLE	LLLE	
LLE	binodal and spinodal points	
GLE		
GLE	gas solubility	
GLE	vapor/gas solubility	
GLE/PVT		
GLE/PVT	gas solubility/density	
GLE/LLE		
GLE/LLE	gas solubility/cloud points	
VLE		
VLE	bubble points	
VLE	partition coefficients	at equilibrium swelling
VLE	partition coefficients	weight fraction based
VLE/LLE		
VLE/LLE	bubble + cloud points	
VLE/GLE		
VLE/GLE	vapor sorption	
SOL		
SOL/SCR	polymer solubility	in supercritical solvent(s)
VLE/SOL		
SWELLING		
LLE/SWELLING		
LLE/SWELLING	partition coefficients	at equilibrium swelling
LLE/SWELLING		
VLE		
VLE	coexistence data	LLV 2 LV und LV 2 LLV
CRI		other critical data
LLE/CRI		
LLE/CRI	cloud points, critical data	
deltaHmix	heat of mixing (general)	
deltaHmix	intermediary enthalpy of dilution [J/mol solvent]	

Currently Polymer-DDB contains 52 different property fields.
Data sets can contain any number and combination of property fields.

Comments can be entered for the data set and each data point

Temperature

Critical temperature (LL > L)

Cloud point temperature

Spinodal temperature

Binodal temperature

Glass Transition Temperature

dT/dP, cloud points

dT/dx, cloud points

.delta.T, (T-TCRIT)

Pressure

Bubble Pressure

Dew Pressure

Density/Volume

Phase Volume Ratio

Specific Volume

Excess Volume

Partial Excess Volume

Partial Excess Volume at inf. Dilution

Intermediary Change of Volume (dilution)

Swelling

Volume Expansion

Concentration

Concentration Range (from)

Concentration Range (to)

Start Concentration

End Concentration

Molecular Weight (GPC)
Molecular Weight (MW)
Molecular Weight (MN)
Molecular Weight (MZ)
Segment Number

Activity
Henry Coefficient (P/W)
Henry Coefficient (P/X)
Henry Coefficient (P/C)
Ostwald Coefficient (V(G)/V(L))
Solubility
Partition Coefficient

Enthalpy of Mixing
Heat of Dilution

Interfacial Tension
dynamic Viscosity
kinematic Viscosity
Shear Rate
Diffusion Coefficient

Reaction Rate
Time

Qualifier
Further Information
pH-value

Fully Integrated
into DDBSP

Dortmund Data Bank (DDB) by DDBST GmbH

File Edit Help

Query Single Sets Selectivity (ACT)

Number	Type/Count	Loc.	Remove	Name
[8]	P	DDB	Remove	[polypropylene]

System

Add/Search Component

Add Compound List

Clear System

Search

System (Exact Match)

Query Result [4]

File Edit

POLYMER

All Sets	All Points	All Ref's	Sets	Points	Ref's
374	2121	24	4	76	1

= POLYMER =
Thermodynamic data for polymer containing systems

Set No.	Pts.	Comp's	#DDB	Tmin [K]	Tmax [K]	Pmin [kPa]	Pmax [kPa]	Comment	Ref.No.	Reference
[1495 0 0]	28	3	[C41] [C161] [P8]	n. a.		n. a.		LLE	30117	[30117] [30117] 01i
[1496 0 0]	26	3	[C161] [C368] [P8]	n. a.		n. a.		LLE	30117	[30117] [30117] 01i
[5770 0 0]	14	3	[C41] [C161] [P8]	n. a.		n. a.		GLE	30117	[30117] [30117] 01i
[5771 0 0]	8	3	[C161] [C368] [P8]	n. a.		n. a.		GLE	30117	[30117] [30117] 01i

Ternary Systems

#	System
1	C41 C161 P8
2	C161 C368 P8

C368: 1-Butene

1 dataset/s marked.

Edit Mixture Data - POLYMER Update<FullVersion>

File Edit Call Help

Components

4	P	DDB	Remove	polyethylene
27	C	DDB	Remove	Chlorobenzene

Add
Salt
Replace
Clear
Sets

Reference

Lit#: 43564
Link#: 0

[43564] Wohlfarth C., Plaste Kautschuk, 40, p272-275, 1993

Quick Plot Std. Plot **7 Line/s**

Note

AZD ACT ACM HE VE CPE GLE ELE POW EGLE CRI ESLE AAE **POLYMER**

Polymer Components Polymer Datatypes Polymer Phases Polymer Properties Polymer Units **Dataset**

Data Type 800 VLE//

Constants Polymer/Component Details Comment

Property	Phase	Compound(s)	Unit	Value	Remove?
1 Temperature	0 System	0 All	37 K	393.15	Remove

New Constant

Add Column Add Qualifier Column Delete Column ...

Property	3 [Concentration]...	31 [Activity]...
Phase	1 [Liquid]...	0 [System]...
Compound	1 [Polymer B]...	2 [Component A]...
Unit	2 [weight fraction]...	73 [P(I)/PSAT(I)]...
1	0.6021	0.7425
2	0.6418	0.6914
3	0.6673	0.6777
4	0.7021	0.6202

Dataset Number 1

Private DDB: Load, Replace, Append, Remove (F10-F12)

DDBST DDB: Load, Replace, Append, Remove (F6-F8)

File: Open (F4), Save (F5)

Find Removed Set: Private DDB, DDBST DDB

Block Write Access to ...
 Private Databases
 Public Databases

Public Sets (C:\DDBMAIN\Ddb\): 14709 Private Sets (C:\DDBMAIN\PRVY\): 0 Hint:

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