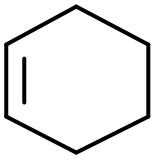
GDF DATA BANKS BULLETIN , VOL. 2 , No. 4 (1998)

VAPORSAT©

DATA BANKS OF THERMALLY DRIVEN VLE
code : VAPORSAT–01©

VOLUME 1 : THE FIRST 100 SIMPLE MOLECULES

standard example of an item :

Cyclohexene ; Tetrahydrobenzene	code	vaporsat–01©
(structure's window) 	RMM	82.15
	EF	C6H10
	CAS	110–83–8
	BRN	906737
	EC	2038078
	MP	169.638
references: 1 – 5	NBP	356.129

UNIVERSAL		ARRHENIUS	
N	5.9522 ± 0.0002	E , kJ/mol	34.2 ± 0.3
–M	26.73 ± 0.05	ln(po)	16.2 ± 0.1
To	163.7 ± 0.1	po	1.04E07 ± 1E06
U–range	213.2 – 423.2	FOM	16.5
FOM	287	m	22

see for details in **GDF DATA BANKS BULLETIN , VOL.3 , NO.1 (1999)**

orders :

- BY SIMPLY PAYING 48 USD IN OUR BANK ACCOUNT (see the inside cover) , OR BY INTERNATIONAL CHEQUE.
- YOU CAN ASK PRIOR FOR THE PROFORMA INVOICE .
- THE PRICE CONTAINS ALL TAXES (INCLUDING SHIPMENT).

VAPORSAT©

DATA BANKS OF VAPOR-LIQUID SEPARATION KINETICS

Vapor-liquid separation kinetics (VLSK) represents in fact the key topic of the vapor-liquid equilibria (VLE) [1,2] with wide practical applications. We must mention that the previous comments on **DIFFUTOR©** [3] are perfect valid for these new databanks.

VAPORSAT© represent databanks of VLSK taking into account basic experimental data as obtained according to topoenergetic requirements and by considering a large variety of driving potentials.

VAPORSAT©-01 represent databanks of VLSK considering temperature as the driving potential, similar with **DIFFUTOR©-01**[3].

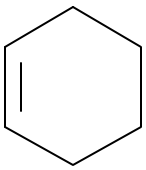
The first volume in this series contains in most condensed form the UNIVERSAL and Arrhenius basic parameters for 106 items grouped I the following categories:

chapter	Category of compounds	No. of items
1	Atomic gases	4
2	Small molecules	12
3	Alkanes	20
4	Olefins	20
5	Cycloalkanes	7
6	Cycloolefins	2
7	Aromatic hydrocarbons	17
8	Alcohols	7
9	C-O-C, C=O compounds	11
10	Cl-hydrocarbons	4
11	N-hydrocarbons	2

Table below gives all details about **VAPORSAT©-01** databank and reproduces a typical example. We must mention again that these simple and pure compounds reveal a specific behaviour of VLSK which very few depends on experimental conditions, so that this databank can be considered as reference data for more complex samples (mixtures), but rigorously requiring the same standard operating procedure.

Typical format of **VAPORSAT©-01** databank does not contain values of correlation coefficient for the two constitutive kinetic equations (UNIVERSAL and Arrhenius representations of the basic experimental data), because the values of FOM(N) and FOM(E) are more suggestive [4].

Assignments of data enclosed for each item in **VAPORSAT©-01** databank

			CYCLO-OLEFINS
Cyclohexene ; Tetrahydrobenzene (name)		**code**	**VAPORSAT©-01**
(structure's window) 		RMM	82.15
		EF	C6H10
		CAS	110–83–8
		BRN	906737
		EC	2038078
		MP	169.638
references: 1 , 4 , 5 , 13		NBP	356.129
UNIVERSAL		**ARRHENIUS**	
N	5.9522 ± 0.0002	E , kJ/mol	34.2 ± 0.3
–M	26.73 ± 0.05	ln(po)	16.2 ± 0.1
To	163.7 ± 0.1	po	1.04E07 ± 1E06
U–range	213.2 – 423.2	FOM	16.5
FOM	287	m	22

- (name): standard (CAS), commercial and/or registered names of the item;
- **code**: the trading code of the data bank for the UNIVERSAL and ARRHENIUS representations, including the standard operating procedure;
- RMM: relative molecular mass of the item in the gas phase;
- EF: empirical molecular formula;
- CAS: Chemical Abstract Registry Number of the item;
- BRN: Beilstein Registry Number of the item;
- EC: European Community Registry Number (EINECS or ELINCS);
- MP: melting point (Kelvin);
- NBP: normal boiling point (Kelvin) (at 101.3 kPa=1 atm);
- references: literature source for experimental data ;
- UNIVERSAL representation of equilibrium pressure of saturated vapor of the item, p (in kPa), at the equilibrium temperature (U=T ,in Kelvin) according to the Universal kinetic equation :

$$\ln p = N * \ln(T - To) + M \qquad (1);$$

- To: freezing point below which the vaporization of the item is inhibited (in Kelvin);
- U-range: temperature range of the experiments (in Kelvin) ;
- FOM (Universal) = Figure of Merit of the considered experiments = 1/((degrees of freedom)*(experimental uncertainty of N));
- E (in kJ/mol): activation energy of the vapor-liquid separation process according to the following kinetic equation:

$$\ln p = -(E / (R*T)) + \ln po \qquad (2);$$

- FOM(Arrhenius)=100/((degrees of freedom)*(experimental uncertainty of E));
- m: number of experiments considered in both representations.

We must mention the same concluding remarks as for DIFFUTOR©-01 and repeat that calorimetric procedures (for instance VDC-4) ensure standard operating procedures for high quality databanks on VLSK allowing to establish higher phylogenies.

References

[1] Gh. Dragan, Behaviour in vapor-liquid equilibria. I. Structural aspects, GDF Databanks Bulletin, 2(1), 3-27 (1998).
[2] Gh. Dragan, Behaviour in vapor-liquid equilibria. I. Several structures in databanks, GDF Databanks Bulletin, 2(1), 27-53 (1998).
[3] **DIFFUTOR©:** Databanks of diffusion kinetics, GDF Databanks Bulletin, 3(1), 3-15 (1999).
[4] **Curs Practic de Metrologie,** GDF Databanks Bulletin, **2S**(2), (1999); **Discussions on Applied Metrology,** GDF Databanks Bulletin, **3**(2), (1999); **Measurement and Calibration,** GDF Databanks Bulletin, **4**(2), (2000).