

# Pure Component Property Estimation Methods of Rarey-Nannoolal

## Introduction:

Several pure component property estimation methods were developed within MSc- and PhD-projects in the group of Prof. Ramjugernath at the University of Kwazulu-Natal (UKZN) in Durban, South Africa. The work was closely supervised by Jürgen Rarey within his position as honorary Prof. at UKZN. DDBST GmbH (Oldenburg) supplied data from the DDB and software support. Development was performed using the software-package ARTIST.

This document gives a brief description of the Rarey-Nannoolal methods. The estimation of the vapor pressure by the Rarey-Moller method is covered in a different document.

Since the publication of the method, numerous small corrections and improvements were added and the model parameter parameters have been refitted several times during this process.

Work on the methods is continued and several further methods have been developed but not yet published.

The methods are described in detail in the references below. In addition, short reproductions of the equations and parameter tables for the estimation of the normal boiling point can be found in e.g. "Perry's Chemical Engineer's Handbook" or the German "VDI-Wärmeatlas".

## References:

Estimation of Pure Component Properties. Part 1. Estimation of the Normal Boiling Point of Non-Electrolyte Organic Compounds via Group Contributions and Group Interactions	Nannoolal Y., Rarey J., Ramjugernath D., Cordes W.	Fluid Phase Equilib., 226, 1, 45-63 (2004)
Estimation of pure component properties Part 2. Estimation of critical property data by group contribution	Nannoolal Y., Rarey J., Ramjugernath J.	Fluid Phase Equilib., 252, 1-2, 1-27 (2007)
Estimation of pure component properties: Part 3. Estimation of the vapor pressure of non-electrolyte organic compounds via group contributions and group interactions	Nannoolal Y., Rarey J., Ramjugernath D.	<a href="#">Fluid Phase Equilib., 269(1-2), 117-133 (2008)</a>
Estimation of pure component properties. Part 4: Estimation of the saturated liquid viscosity of non-electrolyte organic compounds via group contributions and group interactions	Nannoolal Y., Rarey J., Ramjugernath D.	<a href="#">Fluid Phase Equilib., 281 (2), 97-119 (2009)</a>
Estimation of the vapour pressure of non-electrolyte organic compounds via group contributions and group interactions	Moller B., Rarey J., Ramjugernath D.	<a href="#">J.Mol.Liq., 143, 1, 52-63 (2008)</a>

The work is based on a previous method by Rarey and Cordes:

A new method for the estimation of the normal boiling point of non-electrolyte organic compounds	Cordes W., Rarey J.	Fluid Phase Equilib., 201, 19, 409-433 (2002)
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Further published methods are based on a similar approach:

Group Contribution Prediction of Surface Charge Density Profiles for COSMO-RS(OI)	Mu T., Rarey J., Gmehling J.	AIChE J., 53, 12, 3231-3240 (2007)
Group Contribution Prediction of Surface Charge Density Distribution of Molecules for COSMO-SAC	Mu T., Rarey J., Gmehling J.	AIChE J., 55, 12, 3298-3300 (2009)

Additional methods have been developed but are not yet published. These methods are available via the DDBST-Software ARTIST.

- Activity of Complex Molecules in Water (Solubility, ...) (Moller, Rarey, Ramjugernath)
- Activity of Complex Molecules in Alkanes (Solubility, ...) (Moller, Rarey, Ramjugernath)
- Surface Tension (Olivier, Rarey, Ramjugernath)
- Thermal Conductivity (Govender, Rarey, Ramjugernath)

## Group Contribution Scheme

In case of the normal boiling temperature both data for a large number of components are available and a detailed group fragmentation scheme is required. The reason for the latter lies in the fact that at this relatively low temperature, the chemical potential of the molecules in the liquid phase is strongly influenced by energetic and structural effects. In contrast, estimation of the critical temperature could be based on a more simple fragmentation as some structural effects are not important at this much higher temperature and lower density of the fluid.

The group fragmentation scheme was thus developed for normal boiling point estimation and later used for further properties. The list of groups for the estimation methods for the normal boiling temperature is given in the following table:

Group definitions (ID- identification number, PR - priority)

- Abbreviations: (e) - very electronegative neighbors (N, O, F, Cl)  
 (ne) - not very electronegative neighbors (not N, O, F, Cl)  
 (na) - non-aromatic atom or neighbor  
 (a) - aromatic atom or neighbor  
 (c) - atom or neighbor is part of a chain  
 (r) - atom or neighbor is part of a ring

Group	Description	Name	ID PR	occurs e.g. in
Periodic Group				
17				
Fluorine				
F-	F- connected to C or Si	F-(C,Si)	19 86	2-fluoropropane, trimethylfluorosilane

	F- connected to a C or Si already substituted with one F or Cl and one other atom	F-(C-([F,Cl]))-a	22 83	1-chloro-1,2,2,2-tetrafluoroethane[R124], difluoromethylsilane
	F- connected to C or Si already substituted with at least one F and two other atoms	F-(C-([F,Cl]))-b	21 80	1,1,1-trifluoroethane 2,2,3,3-tetrafluoropropionic acid
	F- connected to C or Si already substituted with at least one Cl and two other atoms	F-(C-(Cl))-b	102 81	trichlorofluoromethane[R11], 1,1-dichloro-1-fluoroethane [R141B]
	F- connected to C or Si already substituted with two F or Cl	F-(C-([F,Cl]2))	23 82	1',1',1'-trifluorotoluene, 2,2,2-trifluoroethanol, trifluoroacetic acid
	F- connected to an aromatic carbon	F-(C(a))	24 85	Fluorobenzene, 4-fluoroaniline
	F- on a C=C (vinylfluoride)	-CF=C<	20 84	vinyl fluoride, trifluoroethene, perfluoropropylene
<b>Chlorine</b>				
Cl-	Cl- connected to C or Si not already substituted with F or Cl	Cl- (C,Si)	25 72	butyl chloride, 2-chloroethanol, chloroacetic acid
	Cl- connected to C or Si already substituted with one F or Cl	Cl-((C,Si)-([F,Cl]))	26 71	Dichloromethane, dichloroacetic acid, dichlorosilane
	Cl- connected to C or Si already substituted with at least two F or Cl	Cl-((C,Si)-([F,Cl]2))	27 69	ethyl trichloroacetate, trichloroacetoneitrile
	Cl- connected to an aromatic C	Cl-(C(a))	28 73	chlorobenzene
	Cl- on a C=C (vinylchloride)	-CCl=C<	29 70	vinyl chloride
COCl-	COCl- connected to C (acid chloride)	COCl-	77 19	acetyl chloride, phenylacetic acid chloride
<b>Bromine</b>				
Br-	Br- connected to a non-aromatic C or Si	Br-(C/Si(na))	30 66	ethyl bromide, bromoacetone
Br-	Br- connected to an aromatic C	Br-(C(a))	31 67	bromobenzene
<b>Iodine</b>				
I-	I- connected to C or Si	I-(C,Si)	32 64	ethyl iodide 2-iodotoluene

Periodic Group 16				
Oxygen				
-OH	-OH for aliphatic chains with less than five C (cannot be connected to aromatic fragments)	-OH short chain < C <sub>5</sub>	36 91	ethanol, propanediol
	-OH connected to C or Si substituted with one C or Si in an at least five C or Si containing chain (primary alcohols)	-OH > C <sub>4</sub>	35 87	1-nonanol, tetrahydrofurfuryl alcohol, ethylene cyanohydrin
	-OH connected to a C or Si substituted with two C or Si in a at least three C or Si containing chain (secondary alcohols)	HO-((C,Si) <sub>2</sub> H-(C,Si)-(C,Si)-)	34 89	2-butanol, cycloheptanol
	-OH connected to C which has 4 non hydrogen neighbors (tertiary alcohols)	-OH tert	33 90	tert-butanol, diacetone alcohol
	-OH connected to an aromatic C (phenols)	-OH (Ca)	37 88	phenol, methyl salicylate
-O-	-O- connected to 2 neighbors which are each either C or Si (ethers)	(C,Si)-O-(C,Si)	38 93	diethyl ether, 1,4-dioxane
	-O- in an aromatic ring with aromatic C as neighbors	(C(a))-O(a)- (C(a))	65 92	furan, furfural
-CHO	CHO- connected to non-aromatic C (aldehydes)	CHO-(Cna)	52 53	acetaldehyde, pentanedial
	CHO- connected to aromatic C (aldehydes)	CHO-(Ca)	90 52	Furfural, benzaldehyde
>C=O	-CO- connected to two non-aromatic C, (ketones)	O=C<(Cna) <sub>2</sub>	51 55	acetone, methyl cyclopropyl ketone
	-CO- connected to two C with at least one aromatic C (ketones)	(O=C<(C) <sub>2</sub> )a	92 54	acetophenone, benzophenone
	-CO connected to N	>N(C=O)-	109 39	methyl thioacetate
	-CO connected to two N (urea)	>N-(C=O)-N<	100 2	Urea-1,1,3,3-tetramethyl
O=C(-O-) <sub>2</sub>	Non-cyclic carbonate	O=C(-O-) <sub>2</sub>	79 15	dimethyl carbonate
COOH -	-COOH connected to C	COOH -(C)	44 24	acetic acid

-COO -	HCOO- connected to C (formic acid ester)	HCOO -(C)	46 27	ethyl formate, phenyl formate
	-COO- connected to two C (ester)	(C)-COO -(C)	45 25	ethyl acetate, vinyl acetate
	-COO- in a ring, C is connected to C (lactone)	-C(c)OO-	47 26	$\epsilon$ -caprolactone, crotonolactone
-OCOO-	-CO connected to two O (Carbonates)	-OCOO-	103 34	propylene carbonate 1,3 dioxolan-2-one
-OCON<	-CO connected to O and N (carbamate)	-OCON<	99 1	Trimethylsilyl methylcarbamate
>(OC2)<	>(OC2)< (epoxide)	>(OC2)<	39 50	propylene oxide
-CO-O-CO-	anhydride connected to two C	-C=O-O-C=O-	76 12	acetic anhydride, butyric anhydride
	cyclic anhydride connected to two C	(-C=O-O-C=O-)r	96 11	maleic anhydride, phthalic anhydride
-O-O-	Peroxide	-O-O-	94 32	di-tert-butylperoxide
<b>Sulphur</b>				
-S-S-	-S-S- (disulfide) connected to two C	(C)-S-S-(C)	55 51	dimethyldisulfide, 1,2-dicyclopentyl-1,2-disulfide
-SH	-SH connected to C (thioles)	SH-(C)	53 74	1-propanethiol
-S-	-S- connected to two C	(C)-S-(C)	54 75	methyl ethyl sulfide
	-S- in an aromatic ring	-S(a)-	56 76	thiazole, thiophene
-SO2-	Non-cyclic sulfone connected to two C (sulfones)	(C)-SO2-(C)	82 18	sulfolane, divinylsulfone
>SO <sub>4</sub>	S(=O) <sub>2</sub> connected to two O (sulfates)	>SO <sub>4</sub>	104 35	dimethyl sulfate
-SO <sub>2</sub> N<	-S(=O) <sub>2</sub> connected to N	-SO <sub>2</sub> N<	105 36	N,N-diethylmethanesulfonamide
>S=O	Sulfoxide	>S=O	107 37	1,4-thioxane-S-oxide tetramethylene sulfoxide
SCN-	SCN- (thiocyanate) connected to C	SCN-(C)	81 20	allyl isothiocyanate
<b>Selenium</b>				
>Se<	>Se< connected to atleast 1 C or Si	>Se<	116 46	dimethyl selenide
<b>Periodic Group 15</b>				
<b>Nitrogen</b>				
NH2-	NH2- connected to either C or Si	NH2-(C,Si)	40 95	hexylamine, ethylenediamine
	NH2- connected to an aromatic C	NH2- (Ca)	41 94	aniline, benzidine

-NH-	-NH- connected to 2 neighbors which are each either C or Si (secondary amines)	(C,Si)-NH-(C,Si)	42 99	diethylamine, diallyl amine
	-NH- connected to 2 C or Si neighbors, with atleast 1 aromatic neighbor (secondary amines)	(C,Si)a-NH-(Ca,Si)a	97 98	morpholine pyrrolidine
>N<	>N- connected to 3 neighbors which are each either C or Si (tertiary amines)	(C,Si) <sub>2</sub> >N-(C,Si)	43 100	N,N-dimethylaniline, nicotine
	Quaternary amine connected to 4 C or Si	(C,Si) <sub>2</sub> >N<(C,Si) <sub>2</sub>	101 33	N,N,N,N- tetramethylmethylenediamine
=N-	double bonded amine connected to atleast 1 C or S	(C,Si)=N-	91 101	Acetonin
-N-	aromatic -N- in a 5 membered ring, free electron pair	=N(a)- (r5)	66 97	piperidine, thiazole
=N-	aromatic =N- in a 6 membered ring	=N(a)- (r6)	67 96	pyridine, nicotine
C≡N-	-C≡N (cyanide) connected to C	(C)-C≡N	57 56	acetonitrile, 2,2'-dicyano diethyl sulfide
	-C≡N (cyanide) connected to N	(N)-C≡N	111 41	dimethylcyanamide
	-C≡N (cyanide) connected to S	(S)-C≡N	108 38	methyl thiocyanate
CNCNC-r	imidazole	..=CNC=NC=..	106 3	1 methyl 1 imadizole
-CONH<	-CONH <sub>2</sub> (amide)	-CONH <sub>2</sub>	50 28	acetamide
	-CONH- (monosubstituted amide)	-CONH-	49 48	N-methylformamide, 6-caprolactam
	-CON< (disubstituted amide)	-CON<	48 49	N,N-dimethylformamide (DMF)
OCN-	OCN- connected to C or Si (cyanate)	OCN-	80 29	butylisocyanate, hexamethylene diisocyanate
ONC-	ONC- (oxime)	ONC-	75 30	methyl ethyl ketoxime
-ON=	-ON= connected to C or Si (isoazole)	-ON=(C,Si)	115 45	isoazole 5-phenyl isoazole
NO <sub>2</sub> -	nitrites (esters of nitrous acid)	O=N-O-(C)	74 23	ethyl nitrite, nitrous acid methyl ester
	NO <sub>2</sub> - connected to aliphatic C	NO <sub>2</sub> -(C)	68 21	1-nitropropane
	NO <sub>2</sub> - connected to aromatic C	NO <sub>2</sub> -(C(a))	69 22	nitrobenzene

NO3-	nitrate (esters of nitric acid)	NO3-	72 14	N-butyl nitrate, 1,2-propanediol dinitrate
Phosphorous				
>P(O)-3	phosphates with four O substituents	PO(O)-3	73 10	triethyl phosphate, tris-(2,4-dimethylphenyl) phosphate
>P<	phosphorus connected to at least 1 C or S (phosphine)	>P<	113 43	triphenylphosphine triethylphosphane
Arsine				
AsCl2-	AsCl2 connected to C	AsCl2-	84 17	ethylarsenic dichloride
Periodic Group 14				
Carbon				
-CH3	CH3- not connected to either N, O, F or Cl	CH3-(ne)	1 104	decane
	CH3- connected to either N, O, F or Cl	CH3-(e)	2 102	dimethoxymethane, methyl butyl ether
	CH3- connected to an aromatic atom (not necessarily C)	CH3-(a)	3 103	toluene, p-methyl-styrene
-CH2-	-CH2- in a chain	-C(c)H2-	4 111	butane
	-CH2- in a ring	-C(r)H2-	9 112	cyclopentane
>CH-	>CH- in a chain	>C(c)H-	5 117	2-methylpentane
	>CH- in a ring	>C(r)H-	10 116	methylcyclohexane
>C<	>C< in a chain	>C(c)<	6 119	neopentane
	>C< in a chain connected to at least one aromatic carbon	>C(c)<(a)	8 108	ethylbenzene, diphenylmethane
	>C< in a chain connected to at least one F, Cl, N or O	>C(c)<(e)	7 107	ethanol
	>C< in a ring	>C(r)<	11 118	beta-pinene
	>C< in a ring connected to at least one aromatic carbon	>C(r)<(Ca)	14 106	indene, 2-methyl tetralin
	>C< in a ring connected to at least one N or O which are not part of the ring or one Cl or F	>C(r)<(e,c)	12 109	cyclopentanol, menthol
	>C< in a ring connected to at least one N or O which are part of the ring	>C(r)<(e,r)	13 110	morpholine, nicotine
=C(a)<	aromatic =CH-	=C(a)H-	15 105	benzene

	aromatic =C< not connected to either O,N,Cl or F	=C(a)<(ne)	16 115	ethylbenzene, benzaldehyde
	aromatic =C< with 3 aromatic neighbors	(a)=C(a)<2(a)	18 114	naphthalene, quinoline
	aromatic =C< connected to either O,N,Cl or F	=C(a)<(e)	17 113	aniline, phenol
>C=C<	H2C=C< (1-ene)	H2C(c)=C<	61 58	1-hexene
	>C=C< (both C have at least one non-H neighbor)	>C(c)=C(c)<	58 63	2-heptene, mesityl oxide
	non-cyclic >C=C< connected to at least one aromatic C	>C(c)=C(c)<(C(a))	59 60	isosafole, cinnamic alcohol
	cyclic >C=C<	>C(r)=C(r)<	62 61	cyclopentadiene
	non-cyclic >C=C< substituted with at least one F, Cl, N or O	-(e)C(c)=C(c)<	60 59	trans-1,2-dichloroethylene, perfluoroisoprene
-C≡C-	HC≡C- (1-ine)	HC≡C-	64 57	1-heptyne
	-C≡C-	-C≡C-	63 62	2-octyne
>C=C=C<	cumulated double bond	>C=C=C<	87 6	1,2 butadiene dimethyl allene
>C=C-C=C<	conjugated double bond in a ring	>C=C-C=C<	88 7	cyclopentadiene abietic acid
>C=C-C=C<	conjugated double bond in a chain	>C=C-C=C<	89 8	isoprene 1,3 hexadiene
-C≡C-C≡C-	conjugated triple bond	-C≡C-C≡C-	95 9	2,4 hexadiyne
<b>Silicon</b>				
>Si<	>Si<	>Si<	70 79	butylsilane
	>Si< connected to at least one O	>Si<(O)	71 77	hexamethyl disiloxane
	>Si< connected to at least one F or Cl	>Si<(F,Cl)	78 16	trichlorosilane,
<b>Germanium</b>				
>Ge<	>Ge< connected to four carbons	(C)2>Ge<(C)2	86 68	tetramethylgermane
GeCl3-	GeCl3- connected to carbons	GeCl3-	85 13	fluorodimethylsilyl(trichlorogermanyl)methane
<b>Stannium</b>				
>Sn<	>Sn< connected to four carbons	(C)2>Sn<(C)2	83 65	tetramethylstannane



Periodic Group 13				
Bor				
B(O-) <sub>3</sub>	Non-cyclic boric acid ester	B(O-) <sub>3</sub>	78 16	triethyl borate
Aluminum				
>Al<	>Al< connected to at least 1 C or Si	>Al<	117 47	triethylaluminum

Special correction contributions were added to account for specific structural properties:

Name	Description	ID	occurs e.g. in
C=C-C=O	-C=O connected to sp <sup>2</sup> carbon	134	Benzaldehyde furfural
(C=O)-C([F,Cl] <sub>2,3</sub> )	Carbonyl connected to carbon with two or more halogens	119	Dichloroacetyl chloride
(C=O)-(C([F,Cl] <sub>2,3</sub> )) <sub>2</sub>	Carbonyl connected to two carbon with two or more halogens each	120	Perfluoro-2-propanone
C-[F,Cl] <sub>3</sub>	Carbon with three halogens	121	1,1,1-Trifluorotoluene
(C) <sub>2</sub> -C-[F,Cl] <sub>2</sub>	Secondary carbon with two halogens	122	2,2-Dichloropropane
No Hydrogen	Component has no hydrogen	123	Perfluoro compounds
One Hydrogen	Component has one hydrogen	124	Nonafluorobutane
3/4 Ring	A three or four-membered non-aromatic ring	125	Cyclobutene
5 Ring	A five-membered non-aromatic ring	126	Cyclopentane
Ortho Pair(s)	Ortho position – counted only once and only if there are no meta or para pairs	127	o-Xylene
Meta Pair(s)	Meta position – counted only once and only if there are no para or ortho pairs	128	m-Xylene
Para Pair(s)	Para position – counted only once and only if there are no meta or ortho pairs	129	p-Xylene
((C=)(C)C-CC <sub>3</sub> )	Carbon-carbon bond with four single bonded and one double bonded carbon neighbor	130	Tert-butylbenzene
C <sub>2</sub> C-CC <sub>2</sub>	Carbon-carbon bond with four carbon neighbors, two on each side	131	Bicyclohexyl
C <sub>3</sub> C-CC <sub>2</sub>	Carbon-carbon bond with five carbon neighbors	132	Ethyl bornyl ether
C <sub>3</sub> C-CC <sub>3</sub>	Carbon-carbon bond with six carbon neighbors	133	2,2,3,3-Tetramethylbutane
Si < (F, Cl, Br, I)	A silicon attached to a halogen atom	217	Trichloroethylsilane

In case of critical data, vapor pressure and viscosity, several changes were introduced:

- Group 82 (sulfolane O=S=O) is now used for sulfones. Sulphur is bonded to two carbon atoms of any type.
- The hydrazine group 99 is now used for secondary amines attached to aromatic carbons/silicons.
- Group 106 (imidazol(ar-5-ring)) is now used for sulfate with one O replaced by... $\text{SO}_3$ ... $\text{S}$ .
- Group 110 (piperidine N-N=O) has been replaced by tertiary amines attached to aromatic carbon.

The parameter files on the book material page (via [www.ddbst.com](http://www.ddbst.com)) each contain a complete list of groups and parameters.

### Treatment of Non-Additive Behavior of Hydrogen-Bonding Groups

In case of groups that can act as H-bond donors or acceptors, adding a further group of this type often results in competitive effects between different H-bonding sites that lead to non-additivity of the effect of these groups on the physical property to be estimated.

A well-known case is the occurrence of multiple alcohol-groups in one molecule. The table below lists the groups considered to be non-additive:

Groups considered to be non-additive (group-ID(s) given in brackets)

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A Alcohol (-OH) (34,35,36,37)	J Sulfide (-S(na)-) (54)	M Primary Amine (-NH <sub>2</sub> ) (40, 41)
B Phenol (-OH(a)) (37)	K Aromatic Sulphur (-S(a)-) (56)	N Secondary Amine (>NH) (42,97)
C Carboxylic Acid (-COOH) (44)	L Thiol (-SH) (53)	O Isocyanate (-OCN) (80)
D Ether (-O-) (38)		P Cyanide (-CN) (57)
E Epoxide (>(OC2)<) (39)		Q Nitrate (69)
F Ester (-COOC-) (45,46,47)		R Aromatic N in 5-ring (=N(a)-(r5)) (66)
G Ketone (-CO-) (51,92)		S Aromatic N in 6-ring (=N(a)-(r6)) (67)
H Aldehyde (-CHO) (52,90)		
I Aromatic Oxygen (-O(a)-) (65)		

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Special group interaction parameters  $c_{ij}$  were regressed to account for this behavior. It should be noted that not in every combination this effect is of importance.

## Model Equations

### Estimation of the normal boiling temperature

$$T_B = \frac{(\sum N_i C_i + g_i)}{n^a + b} + c \quad (1)$$

- with  $N_i$  - number of groups of type  $i$   
 $C_i$  - group contribution of group  $i$  [K]  
 $a, b, c$  - adjustable parameters (see parameter file)  
 $n$  - number of atoms in the molecule (except hydrogen)

The total group interaction  $g_i$  can be calculated from the equation

$$GI = \frac{1}{n} \sum_{i=1}^m \sum_{j=1}^m \frac{C_{i-j}}{m-1} \quad (\text{where } C_{i-j} = C_{j-i}) \quad (2)$$

- with  $C_{i-j}$  group interaction contribution between group  $i$  and group  $j$  [K] ( $C_{i-i} = 0$ ),  
 $n$  number of atoms (except hydrogen),  
 $m$  total number of interaction groups in the molecule

To account for the observation, that group interactions become less important for larger molecules, the sum of group interactions is divided by the number of atoms in the molecule (except hydrogen).

In case of a glycerol monoester (2 OH groups, 1 ester group), this results in COH-OH + 2\*COH-ester.

### Estimation of the critical data

$$T_c = T_b \left( b + \frac{1}{a + \left( \sum_i N_i C_i + GI \right)^c} \right) \quad (3)$$

$$\frac{P_c}{kPa} = \frac{(M/(g/mol))^b}{\left( a + \sum_i N_i C_i + GI \right)^2} \quad (4)$$

$$\frac{V_c}{10^{-6} m^3 mol^{-1}} = \frac{\sum_i N_i C_i + GI}{n^a} + b \quad (5)$$

- with
- $T_b$  - normal boiling temperature [K]
  - $N_i$  - number of groups of type i
  - $C_i$  - group contribution of group i
  - $M$  - molecular weight [g/mol]
  - a,b,c - adjustable parameters (see parameter file)
  - n - number of atoms in the molecule (except hydrogen)
  - GI - total group interaction contribution (see above)

### Estimation of the vapor pressure (Rarey-Nannoolal)

$$\log\left(\frac{P^s}{1 atm}\right) = (4.1012 + dB) \left(\frac{T_{rb} - 1}{T_{rb} - \frac{1}{8}}\right) \quad (6)$$

In this equation, the value of  $dB$  does not depend significantly on the normal boiling point or on the units of pressure used. The constant, 4.1012, was computed as a mean value from the correlation of vapor pressure data for several hundred nonpolar components. In this form, the equation can also be applied as an approximation when using  $dB = 0$ . The value of  $dB$  can be estimated using the approach presented in this paper or via an “educated guess” as it is directly correlated with the strength of the intermolecular forces in the mixture.  $dB$  is typically in the range from -0.5 to 2 and is close to zero for non-polar components.

In order to calculate the value of the parameter  $dB$ , the following equation is used:

$$dB = \left(\sum_i N_i C_i + GI\right) - a \quad (7)$$

- where
- $N_i$  - number of groups of type i
  - $C_i$  - group contribution of group i
  - a - adjustable parameter (see parameter file)
  - GI - total group interaction contribution (see above)

### Estimation of the liquid viscosity reference temperature

If no reliable value for the liquid viscosity is available for a component, the temperature at which the component would have a reference viscosity of 1.3 cP can be estimated by the following equation:

$$T_v = aT_b^{0.5} + \frac{\left(\sum_i^M N_i C_i + 2 \cdot GI\right)^b \cdot 1K}{n^c + d} - e \quad (8)$$

with a, b, c, d, e - adjustable parameters (see parameter file)  
T<sub>b</sub> - normal boiling temperature [K]

### Estimation of the temperature dependence of the liquid viscosity

The following equation allows to calculate the viscosity at a temperature T based on the estimated value of dB<sub>v</sub> and the temperature T<sub>v</sub>, at which the liquid has a viscosity of 1.3 cP. If a viscosity is available at a different temperature, this equation can be re-arranged to yield T<sub>v</sub>.

$$\ln\left(\frac{\eta}{1.3cP}\right) = -dB_v \left( \frac{T - T_v}{T - \frac{T_v}{16}} \right) \quad (9)$$

$$dB_v = \frac{\sum_i^M N_i C_i (dB_v)_i + GI}{n^a + b} + c \quad (10)$$

with N<sub>i</sub> - number of groups of type i  
C<sub>i</sub> - group contribution of group i [K]  
dB<sub>v</sub> - viscosity slope parameter  
a,b,c - adjustable parameters (see parameter file)  
n - number of atoms in the molecule (except hydrogen)