

Functional-Segment Activity Coefficient model

Supplementary Material of "Functional-Segment Activity Coefficient model."

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Table 1. Subgroup assignment for typical substances.

Name	CAS	Formula	Count	Subgroup1	nu1	Subgroup2	nu2	Subgroup3	nu3	Subgroup4	nu4
1-BUTENE	106-98-9	C4H8	3	CH3	1	CH2	1	CH2=CH	1		
1-CHLOROBUTANE	109-69-3	C4H9Cl	3	CH3	1	CH2	2	CH2Cl	1		
1-CHLOROHEXANE	0544-10-05	C6H13Cl	3	CH3	1	CH2	4	CH2Cl	1		
1-CHLOROPENTANE	543-59-9	C5H11Cl	3	CH3	1	CH2	3	CH2Cl	1		
1-CHLOROPROPANE	540-54-5	C3H7Cl	3	CH3	1	CH2	1	CH2Cl	1		
1-DECANOL	112-30-1	C10H22O	3	CH3	1	CH2	8	CH2OH	1		
1-DECENE	0872-05-08	C10H20	3	CH3	1	CH2	7	CH2=CH	1		
1-DODECENE	112-41-4	C12H24	3	CH3	1	CH2	9	CH2=CH	1		
1-HEPTANAL	111-71-7	C7H14O	3	CH3	1	CH2	4	CH2CHO	1		
1-HEPTENE	592-76-7	C7H14	3	CH3	1	CH2	4	CH2=CH	1		
1-HEXANAL	66-25-1	C6H12O	3	CH3	1	CH2	3	CH2CHO	1		
1-HEXENE	592-41-6	C6H12	3	CH3	1	CH2	3	CH2=CH	1		
1-NONANAL	124-19-6	C9H18O	3	CH3	1	CH2	6	CH2CHO	1		
1-OCTANAL	124-13-0	C8H16O	3	CH3	1	CH2	5	CH2CHO	1		
1-OCTANOL	111-87-5	C8H18O	3	CH3	1	CH2	6	CH2OH	1		
1-OCTENE	111-66-0	C8H16	3	CH3	1	CH2	5	CH2=CH	1		
1-PENTENE	109-67-1	C5H10	3	CH3	1	CH2	2	CH2=CH	1		
1,1,1-TRICHLOROETHANE	71-55-6	C2H3Cl3	1	CH3CCl3	1						
1,2,3-TRIMETHYLBENZENE	526-73-8	C9H12	3	CH3	3	ACH	3	AC	3		
1,2,4-TRIMETHYLBENZENE	95-63-6	C9H12	3	CH3	3	ACH	3	AC	3		
1,3-BUTADIENE	106-99-0	C4H6	1	CH2=CH	2						
1,3-CYCLOHEXADIENE	592-57-4	C6H8	2	c-CH2	2	c-CH=CH	2				
1,3,5-CYCLOHEPTATRIENE	544-25-2	C7H8	2	c-CH2	1	c-CH=CH	3				
1,3,5-TRIMETHYLBENZENE	108-67-8	C9H12	3	CH3	3	ACH	3	AC	3		
1,4-CYCLOHEXADIENE	628-41-1	C6H8	2	c-CH2	2	c-CH=CH	2				
1,4-PENTADIENE	591-93-5	C5H8	2	CH2	1	CH2=CH	2				
1,5-HEXADIENE	592-42-7	C6H10	2	CH2	2	CH2=CH	2				

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Name	CAS	Formula	Count	Subgroup1	nu1	Subgroup2	nu2	Subgroup3	nu3	Subgroup4	nu4
1,6-HEPTADIENE	3070-53-9	C7H12	2	CH2	3	CH2=CH	2				
2-METHYL-1-BUTANOL	137-32-6	C5H12O	4	CH3	2	CH2	1	CH	1	CH2OH	1
2-METHYL-1-PENTENE	763-29-1	C6H12	3	CH3	2	CH2	2	CH2=C	1		
2-METHYL-1,3-BUTADIENE	78-79-5	C5H8	3	CH3	1	CH2=CH	1	CH2=C	1		
2-METHYL-2-BUTENE	513-35-9	C5H10	2	CH3	3	CH=C	1				
2-METHYLHEPTANE	592-27-8	C8H18	3	CH3	3	CH2	4	CH	1		
2-METHYLHEXANE	591-76-4	C7H16	3	CH3	3	CH2	3	CH	1		
2-METHYLNONANE	871-83-0	C10H22	3	CH3	3	CH2	6	CH	1		
2-METHYLOCTANE	3221-61-2	C9H20	3	CH3	3	CH2	5	CH	1		
2-METHYLPENTANE	107-83-5	C6H14	3	CH3	3	CH2	2	CH	1		
2-OCTANONE	111-13-7	C8H16O	3	CH3	1	CH2	4	CH3COCH2	1		
2,2-DIMETHYLBUTANE	75-83-2	C6H14	3	CH3	4	CH2	1	C	1		
2,2-DIMETHYLPENTANE	590-35-2	C7H16	3	CH3	4	CH2	2	C	1		
2,2,3-TRIMETHYLBUTANE	0464-06-02	C7H16	3	CH3	5	CH	1	C	1		
2,2,4-TRIMETHYLPENTANE	540-84-1	C8H18	4	CH3	5	CH2	1	CH	1	C	1
2,3-DIMETHYLBUTANE	79-29-8	C6H14	2	CH3	4	CH	2				
2,3-DIMETHYLHEPTANE	3074-71-3	C9H20	3	CH3	4	CH2	3	CH	2		
2,3-DIMETHYLHEXANE	584-94-1	C8H18	3	CH3	4	CH2	2	CH	2		
2,3,4-TRIMETHYLPENTANE	565-75-3	C8H18	2	CH3	5	CH	3				
2,4-DIMETHYLPENTANE	0108-08-07	C7H16	3	CH3	4	CH2	1	CH	2		
2,5-DIMETHYLHEXANE	592-13-2	C8H18	3	CH3	4	CH2	2	CH	2		
3-METHYL-1-BUTANOL	123-51-3	C5H12O	4	CH3	2	CH2	1	CH	1	CH2OH	1
3-METHYL-1-BUTENE	563-45-1	C5H10	3	CH3	2	CH	1	CH2=CH	1		
3-METHYLHEPTANE	589-81-1	C8H18	3	CH3	3	CH2	4	CH	1		
3-METHYLHEXANE	589-34-4	C7H16	3	CH3	3	CH2	3	CH	1		
3-METHYLPENTANE	96-14-0	C6H14	3	CH3	3	CH2	2	CH	1		
3,3-DIMETHYLPENTANE	562-49-2	C7H16	3	CH3	4	CH2	2	C	1		
3,3,5-TRIMETHYLHEPTANE	7154-80-5	C10H22	3	CH3	5	CH2	3	CH	2		
4-METHYL-1-PENTENE	691-37-2	C6H12	4	CH3	2	CH2	1	CH	1	CH2=CH	1
4-METHYLHEPTANE	589-53-7	C8H18	3	CH3	3	CH2	4	CH	1		
4-VINYLCYCLOHEXENE	100-40-3	C8H12	4	c-CH2	3	c-CH	1	CH2=CH	1	c-CH=CH	1
5-METHYL-2-HEXANONE	110-12-3	C7H14O	4	CH3	2	CH2	1	CH	1	CH3COCH2	1
ACETALDEHYDE	75-07-0	C2H4O	1	CH3CHO	1						
ACETONE	67-64-1	C3H6O	1	CH3COCH3	1						
ACETOPHENONE	98-86-2	C8H8O	2	ACH	3	CH3COAC3	1				
BENZENE	71-43-2	C6H6	1	ACH	6						
BENZYL ACETATE	0140-11-04	C9H10O2	2	ACH	6	CH3COOCH2	1				

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Name	CAS	Formula	Count	Subgroup1	nu1	Subgroup2	nu2	Subgroup3	nu3	Subgroup4	nu4
BUTYLCYCLOHEXANE	1678-93-9	C10H20	4	CH3	1	CH2	3	c-CH2	5	c-CH	1
CARBON TETRACHLORIDE	56-23-5	CCl4	1	CCl4	1						
CHLOROBENZENE	108-90-7	C6H5Cl	2	ACH	3	CIAC3	1				
CHLOROETHANE	75-00-3	C2H5Cl	2	CH3	1	CH2Cl	1				
CHLOROFORM	67-66-3	CHCl3	1	CHCl3	1						
CIS-1,2-DIMETHYLCYCLOHEXANE	2207-01-04	C8H16	3	CH3	2	c-CH2	4	c-CH	2		
CIS-2-BUTENE	590-18-1	C4H8	2	CH3	2	CH=CH	1				
CIS-2-PENTENE	627-20-3	C5H10	3	CH3	2	CH2	1	CH=CH	1		
CUMENE	98-82-8	C9H12	4	CH3	2	CH	1	ACH	5	AC	1
CYCLOHEPTANE	291-64-5	C7H14	1	c-CH2	7						
CYCLOHEPTENE	628-92-2	C7H12	2	c-CH2	5	c-CH=CH	1				
CYCLOHEXANE	110-82-7	C6H12	1	c-CH2	6						
CYCLOHEXANONE	108-94-1	C6H10O	2	c-CH2	3	c-CH2COCH2	1				
CYCLOHEXENE	110-83-8	C6H10	2	c-CH2	4	c-CH=CH	1				
CYCLOOCTANE	292-64-8	C8H16	1	c-CH2	8						
CYCLOOCTENE	931-88-4	C8H14	2	c-CH2	6	c-CH=CH	1				
CYCLOPENTADIENE	542-92-7	C5H6	2	c-CH2	1	c-CH=CH	2				
CYCLOPENTANE	287-92-3	C5H10	1	c-CH2	5						
CYCLOPENTANONE	120-92-3	C5H8O	2	c-CH2	2	c-CH2COCH2	1				
CYCLOPENTENE	142-29-0	C5H8	2	c-CH2	3	c-CH=CH	1				
DI-N-BUTYL ETHER	142-96-1	C8H18O	3	CH3	2	CH2	4	CH2OCH2	1		
DI-N-BUTYL KETONE	502-56-7	C9H18O	3	CH3	2	CH2	4	CH2COCH2	1		
DI-N-PENTYL ETHER	693-65-2	C10H22O	3	CH3	2	CH2	6	CH2OCH2	1		
DI-N-PROPYL ETHER	111-43-3	C6H14O	3	CH3	2	CH2	2	CH2OCH2	1		
DIETHYL ETHER	60-29-7	C4H10O	2	CH3	2	CH2OCH2	1				
DIETHYL KETONE	96-22-0	C5H10O	2	CH3	2	CH2COCH2	1				
DIETHYL PHTHALATE	84-66-2	C12H14O4	2	CH3	2	AC6H4(CH2COO)2	1				
DIISOBUTYL ETHER	628-55-7	C8H18O	3	CH3	4	CH	2	CH2OCH2	1		
DIISOBUTYL KETONE	108-83-8	C9H18O	3	CH3	4	CH	2	CH2COCH2	1		
DIISOPROPYL ETHER	108-20-3	C6H14O	2	CH3	4	CHOCH	1				
DIMETHYL ETHER	0115-10-06	C2H6O	1	CH3OCH3	1						
DIMETHYL SULFOXIDE	67-68-5	C2H6OS	1	DMSO	1						
DIPROPYL KETONE	123-19-3	C7H14O	3	CH3	2	CH2	2	CH2COCH2	1		
ETHANOL	64-17-5	C2H6O	2	CH3	1	CH2OH	1				
ETHYL ACETATE	141-78-6	C4H8O2	2	CH3	1	CH3COOCH2	1				
ETHYL BENZOATE	93-89-0	C9H10O2	3	CH3	1	ACH	3	CH2COOAC3	1		
ETHYL BUTYRATE	105-54-4	C6H12O2	3	CH3	2	CH2	1	CH2COOCH2	1		

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Name	CAS	Formula	Count	Subgroup1	nu1	Subgroup2	nu2	Subgroup3	nu3	Subgroup4	nu4
ETHYL ISOPROPYL KETONE	565-69-5	C6H12O	2	CH3	3	CH2COCH	1				
ETHYL N-BUTYL ETHER	628-81-9	C6H14O	3	CH3	2	CH2	2	CH2OCH2	1		
ETHYL N-PROPYL KETONE	589-38-8	C6H12O	3	CH3	2	CH2	1	CH2COCH2	1		
ETHYL PROPIONATE	105-37-3	C5H10O2	2	CH3	2	CH2COOCH2	1				
ETHYL PROPYL ETHER	628-32-0	C5H12O	3	CH3	2	CH2	1	CH2OCH2	1		
ETHYL VALERATE	539-82-2	C7H14O2	3	CH3	2	CH2	2	CH2COOCH2	1		
ETHYLBENZENE	100-41-4	C8H10	4	CH3	1	CH2	1	ACH	5	AC	1
ETHYLCYCLOHEXANE	1678-91-7	C8H16	3	CH3	1	c-CH2	6	c-CH	1		
G-BUTYROLACTONE	96-48-0	C4H6O2	1	GBLactone	1						
INDANE	496-11-7	C9H10	3	c-CH2	3	ACH	4	AC	2		
ISOBUTANE	75-28-5	C4H10	2	CH3	3	CH	1				
ISOBUTANOL	78-83-1	C4H10O	3	CH3	2	CH	1	CH2OH	1		
ISOBUTENE	0115-11-07	C4H8	2	CH3	2	CH2=C	1				
ISOBUTYL ACETATE	110-19-0	C6H12O2	3	CH3	2	CH	1	CH3COOCH2	1		
ISOBUTYRALDEHYDE	78-84-2	C4H8O	2	CH3	2	CH2CHO	1				
ISOPENTANE	78-78-4	C5H12	3	CH3	3	CH2	1	CH	1		
ISOPENTYL ACETATE	123-92-2	C7H14O2	4	CH3	2	CH2	1	CH	1	CH3COOCH2	1
ISOPROPANOL	67-63-0	C3H8O	2	CH3	2	CHOH	1				
ISOPROPYL ACETATE	108-21-4	C5H10O2	2	CH3	2	CH3COOCH	1				
ISOPROPYLCYCLOHEXANE	696-29-7	C9H18	4	CH3	2	CH	1	c-CH2	5	c-CH	1
M-XYLENE	108-38-3	C8H10	3	CH3	2	ACH	4	AC	2		
METHANOL	67-56-1	CH4O	1	CH3OH	1						
METHYL ACETATE	79-20-9	C3H6O2	1	CH3COOCH3	1						
METHYL AMYL KETONE	110-43-0	C7H14O	3	CH3	1	CH2	3	CH3COCH2	1		
METHYL ETHYL KETONE	78-93-3	C4H8O	2	CH3	1	CH3COCH2	1				
METHYL ISOBUTYL ETHER	625-44-5	C5H12O	3	CH3	2	CH	1	CH3OCH2	1		
METHYL ISOBUTYL KETONE	0108-10-01	C6H12O	3	CH3	2	CH	1	CH3COCH2	1		
METHYL ISOPROPYL KETONE	563-80-4	C5H10O	2	CH3	2	CH3COCH	1				
METHYL N-BUTYL ETHER	628-28-4	C5H12O	3	CH3	1	CH2	2	CH3OCH2	1		
METHYL N-BUTYL KETONE	591-78-6	C6H12O	3	CH3	1	CH2	2	CH3COCH2	1		
METHYL N-HEPTYL KETONE	821-55-6	C9H18O	3	CH3	1	CH2	5	CH3COCH2	1		
METHYL N-PROPYL KETONE	107-87-9	C5H10O	3	CH3	1	CH2	1	CH3COCH2	1		
METHYL PROPYL ETHER	557-17-5	C4H10O	3	CH3	1	CH2	1	CH3OCH2	1		
METHYL SEC-BUTYL KETONE	565-61-7	C6H12O	3	CH3	2	CH2	1	CH3COCH	1		
METHYL TERT-BUTYL ETHER	1634-04-04	C5H12O	2	CH3	3	CH3OC	1				
METHYLCYCLOHEXANE	108-87-2	C7H14	3	CH3	1	c-CH2	5	c-CH	1		
METHYLCYCLOPENTANE	96-37-7	C6H12	3	CH3	1	c-CH2	4	c-CH	1		

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Name	CAS	Formula	Count	Subgroup1	nu1	Subgroup2	nu2	Subgroup3	nu3	Subgroup4	nu4
N-BUTANE	106-97-8	C4H10	2	CH3	2	CH2	2				
N-BUTANOL	71-36-3	C4H10O	3	CH3	1	CH2	2	CH2OH	1		
N-BUTYL ACETATE	123-86-4	C6H12O2	3	CH3	1	CH2	2	CH3COOCH2	1		
N-BUTYL ETHYL ETHER	628-81-9	C6H14O	3	CH3	2	CH2	2	CH2OCH2	1		
N-BUTYL VALERATE	591-68-4	C9H18O2	3	CH3	2	CH2	4	CH2COOCH2	1		
N-BUTYLBENZENE	104-51-8	C10H14	4	CH3	1	CH2	3	ACH	5	AC	1
N-BUTYRALDEHYDE	123-72-8	C4H8O	3	CH3	1	CH2	1	CH2CHO	1		
N-DECANE	124-18-5	C10H22	2	CH3	2	CH2	8				
N-DOCOSANE	629-97-0	C22H46	2	CH3	2	CH2	20				
N-DODECANE	112-40-3	C12H26	2	CH3	2	CH2	10				
N-DOTRIACONTANE	544-85-4	C32H66	2	CH3	2	CH2	30				
N-EICOSANE	112-95-8	C20H42	2	CH3	2	CH2	18				
N-HEPTANE	142-82-5	C7H16	2	CH3	2	CH2	5				
N-HEXADECANE	544-76-3	C16H34	2	CH3	2	CH2	14				
N-HEXANE	110-54-3	C6H14	2	CH3	2	CH2	4				
N-HEXATRIACONTANE	0630-06-08	C36H74	2	CH3	2	CH2	34				
N-HEXYL ACETATE	142-92-7	C8H16O2	3	CH3	1	CH2	4	CH3COOCH2	1		
N-NONANE	111-84-2	C9H20	2	CH3	2	CH2	7				
N-OCTACOSANE	0630-02-04	C28H58	2	CH3	2	CH2	26				
N-OCTADECANE	593-45-3	C18H38	2	CH3	2	CH2	16				
N-OCTANE	111-65-9	C8H18	2	CH3	2	CH2	6				
N-PENTANE	109-66-0	C5H12	2	CH3	2	CH2	3				
N-PENTANOL	71-41-0	C5H12O	3	CH3	1	CH2	3	CH2OH	1		
N-PENTYL ACETATE	628-63-7	C7H14O2	3	CH3	1	CH2	3	CH3COOCH2	1		
N-PROPANOL	71-23-8	C3H8O	3	CH3	1	CH2	1	CH2OH	1		
N-PROPIONALDEHYDE	123-38-6	C3H6O	2	CH3	1	CH2CHO	1				
N-PROPYL ACETATE	109-60-4	C5H10O2	3	CH3	1	CH2	1	CH3COOCH2	1		
N-PROPYL PROPIONATE	106-36-5	C6H12O2	3	CH3	2	CH2	1	CH2COOCH2	1		
N-PROPYLBENZENE	103-65-1	C9H12	4	CH3	1	CH2	2	ACH	5	AC	1
N-TETRACOSANE	646-31-1	C24H50	2	CH3	2	CH2	22				
N-TETRADECANE	629-59-4	C14H30	2	CH3	2	CH2	12				
N-TETRATRIACONTANE	14167-59-0	C34H70	2	CH3	2	CH2	32				
N-TRIACONTANE	638-68-6	C30H62	2	CH3	2	CH2	28				
N-UNDECANE	1120-21-4	C11H24	2	CH3	2	CH2	9				
NEOPENTANE	463-82-1	C5H12	2	CH3	4	C	1				
O-ETHYLTOLUENE	611-14-3	C9H12	4	CH3	2	CH2	1	ACH	4	AC	2
O-XYLENE	95-47-6	C8H10	3	CH3	2	ACH	4	AC	2		

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P-ETHYLTOLUENE	622-96-8	C9H12	4	CH3	2	CH2	1	ACH	4	AC	2
P-XYLENE	106-42-3	C8H10	3	CH3	2	ACH	4	AC	2		
PROPANE	74-98-6	C3H8	2	CH3	2	CH2	1				
PROPYLENE	0115-07-01	C3H6	2	CH3	1	CH2=CH	1				
SEC-BUTANOL	78-92-2	C4H10O	3	CH3	2	CH2	1	CHOH	1		
SQUALANE	0111-01-03	C30H62	3	CH3	8	CH2	16	CH	6		
TETRAHYDROFURAN	109-99-9	C4H8O	2	c-CH2	2	c-CH2OCH2	1				
TETRAHYDROPYRAN	142-68-7	C5H10O	2	c-CH2	3	c-CH2OCH2	1				
TOLUENE	108-88-3	C7H8	3	CH3	1	ACH	5	AC	1		
TRANS-2-BUTENE	624-64-6	C4H8	2	CH3	2	CH=CH	1				
TRIACETIN	102-76-1	C9H14O6	1	Triacetin	1						
TRIETHYLAMINE	121-44-8	C6H15N	2	CH3	3	N(CH2)3	1				
VALERALDEHYDE	110-62-3	C5H10O	3	CH3	1	CH2	2	CH2CHO	1		
WATER	732-18-5	H2O	1	H2O	1						