CALCULATION OF ABRAHAM MODEL L-DESCRIPTOR AND STANDARD MOLAR ENTHALPIES OF VAPORIZATION FOR LINEAR C_7-C_{14} ALKYNES FROM GAS CHROMATOGRAPHIC RETENTION INDEX DATA

Neel Shanmugam[a], Shrika Eddula[a], William E. Acree Jr[a]* and Michael H. Abraham[b]

Keywords: Linear alkynes, Abraham model, solute descriptors, enthalpy of vaporization, Kovats retention indices.

Abraham model **L** solute descriptors have been determined for an additional 33 linear C_7-C_{14} alkynes based on published gas chromatographic retention indices for solutes eluted from capillary columns coated with squalane and apiezon L stationary phases. Standard molar enthalpies of vaporization and sublimation at 298 K are calculated for the 33 linear alkynes using the reported solute descriptors and our recently published Abraham model correlations. Calculated vaporization enthalpies derived from the Abraham model compare very favourably with values based on a popular atom-group additivity model.

* Corresponding Authors
Fax: (940) 565-3543
E-Mail: acree@unt.edu
[a] Department of Chemistry, University of North Texas, Denton, Texas 76203, USA
[b] Department of Chemistry, University College of London, 20 Gordon Street, London WC1H OAJ, UK

INTRODUCTION

Thousands of new organic and organometallic compounds are either discovered or synthesized each year by the scientific community and chemical manufacturing sector. New chemicals (such as medical drugs, pesticides, herbicides) are synthesized to address specific needs or are discovered during the characterization of chemical constituents of natural products. Practical utilization of newly discovered and newly synthesized compounds requires knowledge of their physical, toxicological and thermodynamic properties. Experimental measurements of properties are often expensive and time-consuming. It is not feasible for experimental measurements to be performed on every newly discovered and newly synthesized organic and organometallic compound. Predictive methods are often used to estimate physical and thermodynamic properties in the absence of measured experimental quantities.

The Abraham solvation parameter model is among the better of the predictive linear free energy relationships developed during the past 30 years. The model has been shown to provide reasonably accurate predictions for a wide range of solute transfer processes. Specific solute properties, *SP*, for which predictive expressions have been reported include: the logarithms of the water-to-organic solvent and gas-to-organic solvent partition coefficients, log *P* and log K,[1-7] logarithms of blood-to-body tissue/fluid partition coefficients, log $P_{blood/tissue}$,[8-12] logarithms of the median lethal concentration of various organic compounds to aquatic organisms, log LC_{50},[13-16] enthalpies of solvation of organic vapors and inorganic gases in organic solvents, ΔH_{solv},[17-27] logarithms of molar solubility ratios,[28-31] isothermal gas chromatographic retention factors and retention indices, *RI*, Draize eye scores and eye irritation thresholds,[32-34] nasal pungency,[32,35-37] skin permeabilities,[38,39] and several other biological response solute properties.[40,41] More recently, the model was successfully extended to the prediction of enthalpies of vaporization[42] and sublimation,[43] vapor pressures of liquid and crystalline organic and organometallic compounds,[44] and isobaric heat capacities.[45]

The popularity of the Abraham model results from the model's simplistic mathematical forms (eqns.1 and 2), coupled with the fact that a single set of solute descriptors (**E**, **S**, **A**, **B**, **V** and **L**) is used in every predictive application. One does not have to compute a different set of solute descriptors for each individual property that one wishes to predict. The common mathematical form that results from having one set of descriptor values facilitates comparisons between the different solute transfer processes using either the Euclidean distance formula or Principal Component Analysis. Such comparisons have been presented in several earlier publications.

$$SP = c_p + e_p \cdot \mathbf{E} + s_p \cdot \mathbf{S} + a_p \cdot \mathbf{A} + b_p \cdot \mathbf{B} + v_p \cdot \mathbf{V} \qquad (1)$$

$$SP = c_k + e_k \cdot \mathbf{E} + s_k \cdot \mathbf{S} + a_k \cdot \mathbf{A} + b_k \cdot \mathbf{B} + l_k \cdot \mathbf{L} \qquad (2)$$

Unlike strictly empirical predictive methods the Abraham model is grounded on a firm understanding of molecular interactions. Each term on the right-hand side of eqns. 1 and 2 represents a different type of solute-solvent interaction that governs solute transfer between two condensed phases, eqn. (1), or solute transfer from the gas phase to a condensed phase, eqn. (2). Molecular interactions are quantified in the Abraham model as the product of a solute descriptor times the complementary condensed phase/solvent property (c_p, e_p, s_p, a_p, b_p, v_p, c_k, e_k, s_k, a_k, b_k, and l_k). Solute descriptors are identified by the uppercase alphabetic characters in eqns. (1) and (2), and are defined as follows: **E** corresponds to the

molar refraction of the given solute in excess of that of a linear alkane having a comparable molecular size, **S** is a combination of the electrostatic polarity and polarizability of the dissolved solute, **A** and **B** quantify the respective hydrogen-bond donating and hydrogen-bond accepting abilities of the solute, **V** refers to the solute's McGowan molecular volume and **L** denotes the logarithm of the solute's measured gas-to-hexadecane partition coefficient at 298.15 K. The lowercase alphabetic characters on the right-hand side of eqns. (1) and (2) denote the complementary properties of the solute transfer process, and their numerical values are determined through regression analysis of experimental partition coefficient data, molar solubility ratios, gas chromatographic retention factors and retention indices, and other measured solute properties as illustrated in earlier publications.[28-31,46-48] Readers are referred to several review articles[49-52] for a more detailed discussion of the Abraham model and its predictive applications.

Continued development of the Abraham model requires determining solute descriptor values for more chemical compounds and developing correlation expressions for additional transfer processes/properties of chemical and biological significance. Our recent efforts in this area have been to publish predictive Abraham model correlations for vapor pressures, enthalpies of vaporization and sublimation and heat capacities of organic and organometallic compounds. Concurrent with developing the fore-mentioned predictive expressions we have calculated solute descriptors for several high-energy nitrogen compounds,[53] several adamantane derivatives[54] and approximately 300 different monoalkylated and polymethylated linear alkanes.[55,56]

The current communication is devoted to obtaining a complete set of solute descriptor values for linear C_7-C_{14} alkynes so that we can predict both their physical and thermodynamic properties. Our private database of solute descriptors has numerical values of **E**, **S**, **A**, **B** and **V** for the complete set of linear $C_7 - C_{14}$ alkynes. **L**-descriptor values, however, are available for only a small fraction of the C_7-C_{14} alkynes. Numerical values of the **E** and **V** solute descriptors, listed in Table 1 were calculated based on the alkynes refractive index and molecular structure (atomic sizes and number of chemical bonds) as described elsewhere[50-52]. The **S**, **A** and **B** descriptors were estimated from known experimental-based values for non-1-yne, dec-1-yne, dodec-1-yne, and the smaller C_4-C_8 alkynes for which a **L**-descriptor value is given. The tabulated values of the **L**-solute descriptors were computed from experimental partition coefficient data. We note that the **S**, **A** and **B** solute descriptors of alkynes are numerically very small, and their contribution to the solute transfer processes defined by eqns. (1) and (2) are also small. The **L** solute descriptor, on the other hand, is much larger and its numerical value cannot be reasonably estimated by comparisons with other linear alkyne molecules. We note that an earlier version of our private solute descriptor database is available on the public UFZ-LSER website[57] (referenced as Abraham Absolv), and that the website will have numerical **L** solute descriptors values for several of the linear alkyne molecules whose solute descriptor values are not given in Table 1. The reference given for the L-descriptor in the website is LSER Dataset 2017 for CompTox users. Numerical values for the **L** solute descriptors referenced as LSER Dataset 2017 might be estimated values based on a derived mathematical correlation between other Abraham model solute descriptors or other estimation scheme. The website for UFZ-LSER Database does have provisions for estimating solute descriptors from a molecule's canonical Smiles code. Our past experience has been that solute descriptors obtained from actual experimental data provide superior predicted values than solute descriptors calculated entirely by estimation methods.

In this study we calculate the **L** solute descriptors of the larger alkyne molecules from the published isothermal gas chromatographic retention index data of Rang and co-workers.[58] The authors measured the retention indices of linear C_6-C_{14} alkynes on capillary columns coated with squalane, apiezon L, polyphenyl ether and polyethylene glycol 4000 stationary phases. The computational methodology will be the same as that used in our two recent papers published in this journal,[55,56] which reported the numerical values of the **L** solute descriptors for approximately 300 large monoalkylated and polymethylated linear alkanes.

CALCULATION OF ABRAHAM MODEL SOLUTE DESCRIPTORS

The computational methodology that we will use to calculate the **L** solute descriptor involves establishing an Abraham model relationship (eqn.3):

$$RI = c_{ri} + e_{ri} \cdot \mathbf{E} + s_{ri} \cdot \mathbf{S} + a_{ri} \cdot \mathbf{A} + b_{ri} \cdot \mathbf{B} + l_{ri} \cdot \mathbf{L} \qquad (3)$$

using the measured Kovats retention indices, *RI*, for those alkane, alkene, and alkynes solutes for which we already have a complete set of solute descriptors. In order to have a sufficient number of experimental data points to establish meaningful Abraham model correlations we augmented the retention index datasets for the squalane and apiezon L stationary phases with experimental values determined by Sojak et al.[59] for linear C_6-C_{14} alkenes on a squalane stationary phase, and with experimental values determined by Vigdergauz et al.[60] and Sojak et al.[61] for several miscellaneous organic compounds on an apiezon L stationary phase. In total we had 100 and 44 experimental data points to use in the regression analyses for constructing the Abraham model correlations for the squalane and apiezon L stationary phases, respectively. The numerical values of the solute descriptors for the alkanes, alkenes and miscellaneous organic compounds used in constructing the Abraham model correlations are tabulated in Table 2. Numerical values of the solute descriptors for the smaller alkyne solutes are listed in Table 1.

We first establish an Abraham model correlation for describing the retention indices of alkane, alkene and alkyne solutes dissolved in the squalane stationary at 110 ºC using the experimental *RI* values given in Table 3. Retention indices of linear alkanes are defined to be 100 times the number of carbon atoms. Squalane (more formally named 2,6,10,15,19,24-hexamethyltetracosane) is a saturated hydrocarbon, and would not be capable of hydrogen-bond formation ($a_k = 0$ and $b_k = 0$) and dipole-dipole interactions ($s_k = 0$). Our published correlation[1] for describing gas-to-liquid partition coefficients into squalane at 298.15 K shows

Table 1. Abraham model solute descriptors of alkynes taken from our private solute descriptor database.

Compound	E	S	A	B	Bo	V	L
But-1-yne	0.178	0.250	0.120	0.100	0.100	0.5862	1.520
But-2-yne	0.261	0.230	0.000	0.210	0.210	0.5862	1.856
Pent-1-yne	0.172	0.230	0.120	0.120	0.120	0.7271	2.010
Pent-2-yne	0.241	0.290	0.000	0.200	0.200	0.7271	2.236
Hex-1-yne	0.166	0.220	0.100	0.120	0.120	0.8680	2.510
Hex-2-yne	0.236	0.300	0.000	0.150	0.150	0.8680	2.765
Hex-3-yne	0.224	0.300	0.000	0.150	0.150	0.8680	2.659
Hept-1-yne	0.160	0.230	0.090	0.100	0.100	1.0089	3.000
Hept-2-yne	0.237	0.300	0.000	0.150	0.150	1.0089	
Hept-3-yne	0.232	0.300	0.000	0.150	0.150	1.0089	
Oct-1-yne	0.155	0.220	0.090	0.100	0.100	1.1498	3.521
Oct-2-yne	0.225	0.300	0.000	0.150	0.150	1.1498	3.850
Oct-3-yne	0.210	0.300	0.000	0.150	0.150	1.1498	
Oct-4-yne	0.208	0.300	0.000	0.150	0.150	1.1498	3.609
Non-1-yne	0.150	0.220	0.090	0.100	0.100	1.2907	4.019
Non-2-yne	0.225	0.300	0.000	0.150	0.150	1.2907	
Non-3-yne	0.204	0.300	0.000	0.150	0.150	1.2907	
Non-4-yne	0.207	0.300	0.000	0.150	0.150	1.2907	
Dec-1-yne	0.143	0.220	0.090	0.100	0.100	1.4316	4.537
Dec-2-yne	0.217	0.300	0.000	0.150	0.150	1.4316	
Dec-3-yne	0.195	0.300	0.000	0.150	0.150	1.4316	
Dec-4-yne	0.205	0.300	0.000	0.150	0.150	1.4316	
Dec-5-yne	0.193	0.300	0.000	0.150	0.150	1.4316	
Undec-1-yne	0.139	0.220	0.090	0.100	0.100	1.5725	
Undec-2-yne	0.213	0.300	0.000	0.150	0.150	1.5725	
Undec-3-yne	0.196	0.300	0.000	0.150	0.150	1.5725	
Undec-4-yne	0.196	0.300	0.000	0.150	0.150	1.5725	
Undec-5-yne	0.191	0.300	0.000	0.150	0.150	1.5725	
Dodec-1-yne	0.133	0.220	0.090	0.100	0.100	1.7134	5.657
Dodec-2-yne	0.207	0.300	0.000	0.150	0.150	1.7134	
Dodec-3-yne	0.190	0.300	0.000	0.150	0.150	1.7134	
Dodec-4-yne	0.190	0.300	0.000	0.150	0.150	1.7134	
Dodec-5-yne	0.190	0.300	0.000	0.150	0.150	1.7134	
Dodec-6-yne	0.190	0.300	0.000	0.150	0.150	1.7134	
Tridec-1-yne	0.136	0.220	0.090	0.100	0.100	1.8543	
Tridec-2-yne	0.209	0.300	0.000	0.150	0.150	1.8543	
Tridec-3-yne	0.209	0.300	0.000	0.150	0.150	1.8543	
Tridec-4-yne	0.209	0.300	0.000	0.150	0.150	1.8543	
Tridec-5-yne	0.209	0.300	0.000	0.150	0.150	1.8543	
Tridec-6-yne	0.209	0.300	0.000	0.150	0.150	1.8543	
Tetradec-1-yne	0.144	0.220	0.090	0.100	0.100	1.9952	
Tetradec-2-yne	0.206	0.300	0.000	0.150	0.150	1.9952	
Tetradec-3-yne	0.206	0.300	0.00	0.15	0.150	1.9952	
Tetradec-4-yne	0.206	0.300	0.000	0.150	0.150	1.9952	
Tetradec-5-yne	0.206	0.300	0.000	0.150	0.150	1.9952	
Tetradec-6-yne	0.206	0.300	0.000	0.150	0.150	1.9952	
Tetradec-7-yne	0.206	0.300	0.000	0.150	0.150	1.9952	

Table 2. Abraham model solute descriptors for alkanes, alkenes and miscellaneous organic compounds.

Compound	E	S	A	B	L	V
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949
Octane	0.000	0.000	0.000	0.000	3.677	1.2358
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767
Decane	0.000	0.000	0.000	0.000	4.686	1.5176
Undecane	0.000	0.000	0.000	0.000	5.191	1.6585
Dodecane	0.000	0.000	0.000	0.000	5.696	1.7994
Tridecane	0.000	0.000	0.000	0.000	6.200	1.9403
Tetradecane	0.000	0.000	0.000	0.000	6.705	2.0812
Pentadecane	0.000	0.000	0.000	0.000	7.209	2.2221
Hexadecane	0.000	0.000	0.000	0.000	7.714	2.3630
Heptadecane	0.000	0.000	0.000	0.000	8.218	2.5039
Octadecane	0.000	0.000	0.000	0.000	8.722	2.6448
Hex-1-ene	0.078	0.080	0.000	0.070	2.572	0.9110
cis-Hex-2-ene	0.143	0.080	0.000	0.070	2.684	0.9110
trans-Hex-2-ene	0.122	0.080	0.000	0.060	2.655	0.9110
cis-Hex-3-ene	0.128	0.080	0.000	0.070	2.664	0.9110
trans-Hex-3-ene	0.126	0.080	0.000	0.060	2.659	0.9110
Hept-1-ene	0.092	0.080	0.000	0.070	3.063	1.0519
cis-Hept-2-ene	0.136	0.080	0.000	0.070	3.210	1.0519
trans-Hept-2-ene	0.119	0.080	0.000	0.070	3.180	1.0519
cis-Hept-3-ene	0.130	0.080	0.000	0.070	3.143	1.0519
trans-Hept-3-ene	0.121	0.080	0.000	0.070	3.125	1.0519
Oct-1-ene	0.094	0.080	0.000	0.070	3.568	1.1928
cis-Oct-2-ene	0.135	0.080	0.000	0.070	3.683	1.1928
trans-Oct-2-ene	0.123	0.070	0.000	0.070	3.668	1.1928
cis-Oct-3-ene	0.125	0.060	0.000	0.070	3.663	1.1928
trans-Oct-3-ene	0.119	0.060	0.000	0.060	3.647	1.1928
cis-Oct-4-ene	0.133	0.080	0.000	0.070	3.607	1.1928
trans-Oct-4-ene	0.114	0.080	0.000	0.070	3.593	1.1928
Non-1-ene	0.090	0.080	0.000	0.070	4.073	1.3337
cis-Non-2-ene	0.136	0.060	0.000	0.060	4.245	1.3337
trans-Non-2-ene	0.119	0.060	0.000	0.060	4.188	1.3337
cis-Non-3-ene	0.127	0.060	0.000	0.060	4.151	1.3337
trans-Non-3-ene	0.119	0.060	0.000	0.060	4.148	1.3337
cis-Non-4-ene	0.132	0.060	0.000	0.060	4.173	1.3337
trans-Non-4-ene	0.116	0.060	0.000	0.060	4.141	1.3337
Dec-1-ene	0.093	0.080	0.000	0.070	4.533	1.4746
cis-Dec-2-ene	0.131	0.060	0.000	0.060	4.745	1.4746
trans-Dec-2-ene	0.118	0.060	0.000	0.060	4.670	1.4746
cis-Dec-3-ene	0.131	0.060	0.000	0.060	4.680	1.4746
trans-Dec-3-ene	0.118	0.060	0.000	0.060	4.671	1.4746
cis-Dec-4-ene	0.131	0.060	0.000	0.060	4.669	1.4746
trans-Dec-4-ene	0.115	0.060	0.000	0.060	4.638	1.4746
cis-Dec-5-ene	0.123	0.060	0.000	0.060	4.665	1.4746
trans-Dec-5-ene	0.112	0.060	0.000	0.060	4.637	1.4746
Undec-1-ene	0.091	0.080	0.000	0.070	5.023	1.6155
cis-Undec-2-ene	0.134	0.060	0.000	0.060	5.258	1.6155
trans-Undec-2-ene	0.117	0.060	0.000	0.060	5.192	1.6155
cis-Undec-3-ene	0.125	0.060	0.000	0.060	5.178	1.6155
trans-Undec-3-ene	0.115	0.060	0.000	0.060	5.150	1.6155
cis-Undec-4-ene	0.129	0.060	0.000	0.060	5.168	1.6155

trans-Undec-4-ene	0.111	0.060	0.000	0.060	5.138	1.6155
cis-Undec-5-ene	0.122	0.060	0.000	0.060	5.153	1.6155
trans-Undec-5-ene	0.095	0.060	0.000	0.060	5.126	1.6155
Dodec-1-ene	0.089	0.080	0.000	0.070	5.515	1.7564
cis-Dodec-2-ene	0.132	0.060	0.000	0.060	5.766	1.7564
trans-Dodec-2-ene	0.116	0.060	0.000	0.060	5.699	1.7564
cis-Dodec-3-ene	0.132	0.060	0.000	0.060	5.692	1.7564
trans-Dodec-3-ene	0.115	0.060	0.000	0.060	5.656	1.7564
cis-Dodec-4-ene	0.123	0.060	0.000	0.060	5.667	1.7564
trans-Dodec-4-ene	0.112	0.060	0.000	0.060	5.641	1.7564
cis-Dodec-5-ene	0.116	0.060	0.000	0.060	5.653	1.7564
trans-Dodec-5-ene	0.092	0.060	0.000	0.060	5.636	1.7564
cis-Dodec-6-ene	0.120	0.060	0.000	0.060	5.655	1.7564
trans-Dodec-6-ene	0.119	0.060	0.000	0.060	5.647	1.7564
Tridec-1-ene	0.093	0.060	0.000	0.070	6.046	1.8973
cis-Tridec-2-ene	0.131	0.060	0.000	0.070	6.261	1.8973
trans-Tridec-2-ene	0.115	0.060	0.000	0.070	6.249	1.8973
cis-Tridec-3-ene	0.122	0.060	0.000	0.070	6.255	1.8973
trans-Tridec-3-ene	0.114	0.060	0.000	0.070	6.249	1.8973
cis-Tridec-4-ene	0.127	0.060	0.000	0.070	6.172	1.8973
trans-Tridec-4-ene	0.111	0.060	0.000	0.070	6.142	1.8973
cis-Tridec-5-ene	0.110	0.060	0.000	0.070	6.146	1.8973
trans-Tridec-5-ene	0.089	0.060	0.000	0.070	6.125	1.8973
cis-Tridec-6-ene	0.119	0.060	0.000	0.070	6.144	1.8973
trans-Tridec-6-ene	0.117	0.060	0.000	0.070	6.144	1.8973
Tetradec-1-ene	0.090	0.060	0.000	0.070	6.536	2.0382
cis-Tetradec-2-ene	0.130	0.060	0.000	0.070	6.840	2.0382
trans-Tetradec-2-ene	0.114	0.060	0.000	0.070	6.743	2.0382
cis-Tetradec-3-ene	0.121	0.060	0.000	0.070	6.755	2.0382
trans-Tetradec-3-ene	0.113	0.060	0.000	0.070	6.719	2.0382
cis-Tetradec-4-ene	0.126	0.060	0.000	0.070	6.776	2.0382
trans-Tetradec-4-ene	0.110	0.060	0.000	0.070	6.731	2.0382
cis-Tetradec-5-ene	0.114	0.060	0.000	0.070	6.753	2.0382
trans-Tetradec-5-ene	0.086	0.060	0.000	0.070	6.696	2.0382
cis-Tetradec-6-ene	0.118	0.060	0.000	0.070	6.762	2.0382
trans-Tetradec-6-ene	0.116	0.060	0.000	0.070	6.726	2.0382
cis-Tetradec-7-ene	0.109	0.060	0.000	0.070	6.734	2.0382
trans-Tetradec-7-ene	0.091	0.060	0.000	0.070	6.713	2.0382
Isopropylbenzene	0.602	0.490	0.000	0.160	4.084	1.1391
Propylbenzene	0.604	0.500	0.000	0.150	4.230	1.1391
1,3,5-Trimethylbenzene	0.649	0.520	0.000	0.190	4.344	1.1391
1,2,4-Trimethylbenzene	0.677	0.560	0.000	0.190	4.441	1.1391
1-Methyl-4-isopropylbenzene	0.607	0.490	0.000	0.190	4.590	1.2800
1,2,3-Trimethylbenzene	0.728	0.610	0.000	0.190	4.565	1.1391
1,2-Diethylbenzene	0.688	0.500	0.000	0.180	4.732	1.2800
1,3-Diisopropylbenzene	0.605	0.460	0.000	0.200	5.170	1.5618
1,2,3,5-Tetramethylbenzene	0.748	0.610	0.000	0.190	5.052	1.2800
1,4-Diisopropylbenzene	0.616	0.470	0.000	0.200	5.315	1.5618
1-Hexanol	0.210	0.420	0.370	0.480	3.610	1.0127
1-Nonanol	0.193	0.420	0.370	0.480	5.120	1.4354
Pentadec-1-ene	0.083	0.060	0.000	0.070	7.008	2.1791
Hexadec-1-ene	0.081	0.080	0.000	0.070	7.586	2.3200

that the squalane solvent does have a non-zero e_k coefficient. Analysis of the *RI* values in Table 3 in accordance with eqn. (3) yielded the following Abraham model expression.

Table 3. Retention indices, r_i (at 383 K) on a squalane stationary phase column, and Abraham model **L** solute descriptors for linear alkanes, alkenes and alkynes.

Compound	*RI*/100	L Value database	L Value Eqn. (5)
Hex-1-yne	5.839	2.510	2.565
Hex-2-yne	6.384	2.765	2.864
Hex-3-yne	6.199	2.659	2.765
Hept-1-yne	6.842	3.000	3.084
Hept-2-yne	7.420		3.402
Hept-3-yne	7.158		3.265
Oct-1-yne	7.837	3.521	3.598
Oct-2-yne	8.418	3.850	3.916
Oct-3-yne	8.163		3.780
Oct-4-yne	8.103	3.609	3.749
Non-1-yne	8.841	4.019	4.118
Non-2-yne	9.406		4.428
Non-3-yne	9.147		4.289
Non-4-yne	9.097		4.264
Dec-1-yne	9.842	4.537	4.635
Dec-2-yne	10.408		4.946
Dec-3-yne	10.131		4.797
Dec-4-yne	10.068		4.767
Dec-5-yne	10.080		4.770
Undec-1-yne	10.842		5.152
Undec-2-yne	11.401		5.460
Undec-3-yne	11.124		5.312
Undec-4-yne	11.048		5.273
Undec-5-yne	11.043		5.269
Dodec-1-yne	11.844	5.657	5.670
Dodec-2-yne	12.398		5.975
Dodec-3-yne	12.114		5.824
Dodec-4-yne	12.033		5.782
Dodec-5-yne	12.017		5.773
Dodec-6-yne	12.003		5.766
Hexane	6.000	2.668	2.609
Heptane	7.000	3.173	3.128
Octane	8.000	3.677	3.646
Nonane	9.000	4.182	4.164
Decane	10.000	4.686	4.683
Undecane	11.000	5.191	5.201
Dodecane	12.000	5.696	5.720
Tridecane	13.000	6.200	6.238
Tetradecane	14.000	6.705	6.756
Pentadecane	15.000	7.209	7.275
Hexadecane	16.000	7.714	7.793
Heptadecane	17.000	8.218	8.312
Octadecane	18.000	8.722	8.830
Hex-1-ene	5.840	2.572	2.545
cis-Hex-2-ene	6.054	2.684	2.671
trans-Hex-2-ene	5.964	2.655	2.619
cis-Hex-3-ene	5.937	2.664	2.607
trans-Hex-3-ene	5.906	2.659	2.590
Hept-1-ene	6.835	3.063	3.064
cis-Hept-2-ene	7.051	3.210	3.186
trans-Hept-2-ene	6.987	3.180	3.149
cis-Hept-3-ene	6.923	3.143	3.118
trans-Hept-3-ene	6.874	3.125	3.091
Oct-1-ene	7.829	3.568	3.579
cis-Oct-2-ene	8.036	3.683	3.696
trans-Oct-2-ene	7.973	3.668	3.661
cis-Oct-3-ene	7.902	3.663	3.625
trans-Oct-3-ene	7.880	3.647	3.612
cis-Oct-4-ene	7.886	3.607	3.618
trans-Oct-4-ene	7.841	3.593	3.590
Non-1-ene	8.828	4.073	4.096
cis-Non-2-ene	9.026	4.245	4.210
trans-Non-2-ene	8.966	4.188	4.175
cis-Non-3-ene	8.881	4.151	4.133
trans-Non-3-ene	8.865	4.148	4.122
cis-Non-4-ene	8.860	4.173	4.123
trans-Non-4-ene	8.844	4.141	4.111
Dec-1-ene	9.827	4.533	4.615
cis-Dec-2-ene	10.022	4.745	4.725
trans-Dec-2-ene	9.966	4.670	4.693
cis-Dec-3-ene	9.864	4.680	4.643
trans-Dec-3-ene	9.855	4.671	4.635
cis-Dec-4-ene	9.834	4.669	4.627
trans-Dec-4-ene	9.827	4.638	4.620
cis-Dec-5-ene	9.821	4.665	4.619
trans-Dec-5-ene	9.847	4.637	4.630
Undec-1-ene	10.826	5.023	5.132
cis-Undec-2-ene	11.019	5.258	5.242
trans-Undec-2-ene	10.965	5.192	5.210
cis-Undec-3-ene	10.858	5.178	5.157
trans-Undec-3-ene	10.853	5.150	5.152
cis-Undec-4-ene	10.811	5.168	5.133
trans-Undec-4-ene	10.812	5.138	5.130
cis-Undec-5-ene	10.789	5.153	5.120
trans-Undec-5-ene	10.820	5.126	5.130
Dodec-1-ene	11.834	5.515	5.654
cis-Dodec-2-ene	12.023	5.766	5.762

trans-Dodec-2-ene	11.969	5.699	5.731
cis-Dodec-3-ene	11.857	5.692	5.676
trans-Dodec-3-ene	11.852	5.656	5.670
cis-Dodec-4-ene	11.806	5.667	5.648
trans-Dodec-4-ene	11.811	5.641	5.648
cis-Dodec-5-ene	11.766	5.653	5.625
trans-Dodec-5-ene	11.811	5.636	5.643
cis-Dodec-6-ene	11.760	5.655	5.623
trans-Dodec-6-ene	11.801	5.647	5.644
Tridec-1-ene	12.835	6.046	6.174
cis-Tridec-2-ene	13.022	6.261	6.280
trans-Tridec-2-ene	12.970	6.249	6.249
cis-Tridec-3-ene	12.851	6.255	6.189
trans-Tridec-3-ene	12.851	6.249	6.187
cis-Tridec-4-ene	12.798	6.172	6.163
trans-Tridec-4-ene	12.803	6.142	6.162
cis-Tridec-5-ene	12.750	6.146	6.134
trans-Tridec-5-ene	12.803	6.125	6.157
cis-Tridec-6-ene	12.725	6.144	6.123
trans-Tridec-6-ene	12.781	6.144	6.152
Tetradec-1-ene	13.832	6.536	6.690
cis-Tetradec-2-ene	14.015	6.840	6.794
trans-Tetradec-2-ene	13.969	6.743	6.767
cis-Tetradec-3-ene	13.841	6.755	6.702
trans-Tetradec-3-ene	13.846	6.719	6.703
cis-Tetradec-4-ene	13.777	6.776	6.670
trans-Tetradec-4-ene	13.793	6.731	6.675
cis-Tetradec-5-ene	13.720	6.753	6.638
trans-Tetradec-5-ene	13.784	6.696	6.664
cis-Tetradec-6-ene	13.686	6.762	6.621
trans-Tetradec-6-ene	13.757	6.726	6.657
cis-Tetradec-7-ene	13.667	6.734	6.609
trans-Tetradec-7-ene	13.745	6.713	6.645

$$RI/100 = 0.967(0.058) - 0.458(0.245)\ \mathbf{E} + 1.929(0.008)\ \mathbf{L} \quad (4)$$

(N = 100, SD = 0.111, R^2 = 0.998, F = 30284)

where N is the number of experimental data points, SD is the standard deviation, R^2 is the squared correlation coefficient, and F is the Fisher F-statistic. Standard errors in the equation coefficients are given in parentheses immediately following the respective coefficient.

We first establish Equation (4) provides a reasonably accurate mathematical description of the gas chromatographic elution behaviour of the 100 alkane, alkene and alkyne solutes on the squalane stationary phase. Through suitable mathematical rearrangement of eqn. (4)

$$\mathbf{L} = [(RI/100) - 0.967 + 0.458\ \mathbf{E}]/1.929 \quad (5)$$

one can calculate the **L** solute descriptors of the remaining 20 C_7-C_{12} alkynes for which *RI* values are available on a squalane stationary phase. The numerical values of our calculated **L** solute descriptors are given in the last column of Table 3. The average error and average absolute error between the **L** values in our database and those calculated based on eqn. (5) are AE = -0.001 and AAE = 0.043, respectively. We do note that the tabulated numerical values of the L solute descriptor based on eqn. (5) differ somewhat from the numerical values given UFZ-LSER Database[57] that are referenced to LSER Dataset 2017.

Rang and coworkders[58] also determined the isothermal Kovats retention indices of linear C_7-C_{14} alkynes on capillary columns coated with apiezon L, polyphenyl ether and polyethylene glycol 4000 stationary phases at elevated temperatures. Of particular interest are the chromatographic measurements for the linear tridecynes and tetradecynes for which we do not have numerical values of the **L** solute descriptors. A search of the published chemical and engineering literature found Kovats retention indices[60,61] for isopropylbenzene, propylbenzene, 1,3,5-trimethylbenzene, 1,2,4-trimethylbenzene, 1-methyl-4-isopropylbenzene, 1,2,3-trimethylbenzene, 1-hexanol, 1,2-diethylbenzene, 1,3-diisopropylbenzene, 1,2,3,5-tetramethylbenzene, 1,4-diisopropylbenzene, 1-pentadecene, 1-hexadecene, 1-heptadecene, and 1-nonanol on an apieizon L stationary phase column at 423 K. Including the retention index data of Rang et al.[58] for the linear decynes, undecynes and dodecynes for which we just computed **L** solute descriptors (see Table 3), there are 44 experimental data points to use in constructing an Abraham model correlation. This should be sufficient to develop a meaningful Abraham model correlation for describing the retention behaviour of organic compounds on an apiezon L stationary phase. It takes between 30 to 40 experimental values to develop an Abraham model correlation.

Analysis of the experimental data in the second column of Table 4 yielded the following Abraham model expression:

$$RI/100 = 0.686(0.066) + 2.788(0.161)\ \mathbf{E} - 2.011(0.199)\ \mathrm{S} + 2.115(0.197)\ \mathrm{A} + 1.988(0.011)\ \mathbf{L} \quad (6)$$

(N = 44, SD = 0.088, R^2 = 0.999, F = 9996)

Preliminary analysis showed that the $b_k \cdot \mathbf{B}$ term made a negligible contribution to the $RI/100$ calculation (with s_k being –0.029) and this term was removed from the final regression. Eqn. (6) provides a reasonably accurate mathematical description of the observed gas chromatographic elution behavior of the 44 organic solutes on the apiezon stationary phase.

$$\mathbf{L} = [(RI/100) - 0.686 - 2.788\ \mathbf{E} + 2.011\ \mathbf{S} - 2.115\ \mathbf{A}]/1.988 \quad (7)$$

Through suitable mathematical rearrangement of eqn. (6), one can calculate the **L** solute descriptors of the linear tridecynes and tetradecynes for which *RI* values are available on an apiezon stationary phase. The numerical values of our calculated **L** solute descriptors are given in the last column of Table 4. The average error and average absolute error between the **L** values in our database and those calculated based on eqn. (5) are AE = 0.001 and AAE

= 0.026, respectively. Solute descriptors for the linear tridecynes and tetradecynes are contained in the UFZ-LSER Database, however, numerical values can be estimated based on the molecule's canonical Smiles code. We were not able to find sufficient *RI* data for solutes eluted from polyphenyl ether and polyethylene glycol 4000 stationary phases to develop Abraham model correlations.

Table 4. Retention indices, *RI* (at 423 K) on an Apiezon L phase column, and Abraham model **L** solute descriptors for linear alkanes, linear alkynes and miscellaneous organic compounds used in the construction of eqn. (7).

Compound	*RI*/100	L Value Database	L Value Eqn. (7)
Dec-1-yne	9.972	4.537	4.597
Dec-2-yne	10.506	4.946	4.939
Dec-3-yne	10.174	4.797	4.803
Dec-4-yne	10.108	4.767	4.755
Dec-5-yne	10.129	4.770	4.783
Undec-1-yne	10.952	5.152	5.096
Undec-2-yne	11.508	5.460	5.448
Undec-3-yne	11.169	5.312	5.302
Undec-4-yne	11.099	5.273	5.267
Undec-5-yne	11.092	5.269	5.270
Dodec-1-yne	11.952	5.657	5.607
Dodec-2-yne	12.505	5.975	5.958
Dodec-3-yne	12.164	5.824	5.811
Dodec-4-yne	12.086	5.782	5.771
Dodec-5-yne	12.074	5.773	5.765
Dodec-6-yne	12.060	5.766	5.758
Tridec-1-yne	12.955		6.108
Tridec-2-yne	13.506		6.459
Tridec-3-yne	13.158		6.284
Tridec-4-yne	13.071		6.240
Tridec-5-yne	13.055		6.232
Tridec-6-yne	13.026		6.218
Tetradec-1-yne	13.957		6.600
Tetradec-2-yne	14.507		6.967
Tetradec-3-yne	14.149		6.787
Tetradec-4-yne	14.069		6.746
Tetradec-5-yne	14.039		6.731
Tetradec-6-yne	14.011		6.717
Tetradec-7-yne	14.002		6.713
Hexane	6.000	2.668	2.673
Heptane	7.000	3.173	3.176
Octane	8.000	3.677	3.679
Nonane	9.000	4.182	4.182
Decane	10.000	4.686	4.685
Undecane	11.000	5.191	5.188
Dodecane	12.000	5.696	5.691
Tridecane	13.000	6.200	6.194
Tetradecane	14.000	6.705	6.697
Pentadecane	15.000	7.209	7.200
Hexadecane	16.000	7.714	7.703
Heptadecane	17.000	8.218	8.206
Octadecane	18.000	8.722	8.709
Isopropylbenzene	9.550	4.084	4.110
Propylbenzene	9.860	4.230	4.273
1,3,5-Trimethylbenzene	10.127	4.344	4.365
1,2,4-Trimethylbenzene	10.370	4.441	4.488
1-Methyl-4-isopropylbenzene	10.540	4.590	4.601
1,2,3-Trimethylbenzene	10.701	4.565	4.634
1,2-Diethylbenzene	10.870	4.732	4.664
1,3-Diisopropylbenzene	11.440	5.170	5.026
1,2,3,5-Tetramethylbenzene	11.690	5.052	5.103
1,4-Diisopropylbenzene	11.880	5.315	5.242
Hexan-1-ol	8.420	3.610	3.627
Nonan-1-ol	11.360	5.120	5.130
Pentadec-1-ene	14.888	7.008	7.088
Hexadec-1-ene	15.881	7.586	7.611
Heptadec-1-ene	16.876	8.031	8.113

[a]Solute descriptors for heptadec-1-ene are: **E** = 0.080; **S** = 0.080; **A** = 0.000; **B** = 0.080; V = 2.4609; and **L** = 8.031

PREDICTION OF MOLAR ENTHALPIES OF VAPORIZATONI OF LINEAR ALKYNES

Now that we have calculated the **L** solute descriptors of C_7-C_{14} linear alkynes we wish to illustrate how the numerical values can be used by the scientific community and manufacturing sector to predict unmeasured physical and chemical properties. Of the properties for which we have reported Abraham model correlations enthalpies of vaporization seem the most logical choice for the linear alkynes. Large alkynes have very limited solubility in water. The likelihood that the scientific community will want to predict the compounds' water-to-organic solvents and lethal molar concentrations towards aquatic organisms is small. Even if large alkynes were to be accidentally released in the environment their aqueous molar concentration would be too small to do significant harm to fish and other aquatic organisms. Large alkynes are not medicinal compounds and there is little demand in the pharmaceutical community to estimate their distribution in the body.

Knowledge of gas chromatographic Kovats retention indices of linear alkynes would aid practical analytical chemists in selecting an appropriate stationary phase to separate alkynes from other hydrocarbons that might be present in petroleum-based samples. These calculations are essentially the reverse of the calculations that we just employed in calculating the **L**-solute descriptors. There would not be much in the way of new information by performing more repetitive-like calculations. After considerable thought we decided to illustrate the practical applications by predicting enthalpies of vaporization as these quantities might be needed in the design of high temperature industrial processes. Enthalpies of vaporization describe how the vapor pressure of a compound varies with temperature.

Our published Abraham model correlation[42] (eqn. 8)

$$\Delta H_{vap,298K}\ (\text{kJ mol}^{-1}) = 6.100 - 7.363\ \mathbf{E} + 9.733\ \mathbf{S} + 4.025\ \mathbf{A} + 2.123\ \mathbf{B} + 9.537\ \mathbf{L} - 1.180\ \mathbf{S}\cdot\mathbf{S} + 77.871\ \mathbf{A}\cdot\mathbf{B} - 5.781\ \mathbf{I}_{amine} - 14.783\ \mathbf{I}_{non\text{-}\alpha,\omega\text{-}diol} - 17.873\ \mathbf{I}_{\alpha,\omega\text{-}diol} \quad (8)$$

(with N = 703, SD = 2.09, R^2 = 0.986, F = 4925.6)

provides reasonably accurate predictions of the standard molar enthalpies of vaporization, $\Delta H_{vap,298K}$, as evidence by the correlation's standard deviations of SD = 2.09 kJ mol^{-1}, which is slightly larger than the experimental uncertainty associated with the measured $\Delta H_{vap,298K}$, values. For the linear C_7-C_{14} alkynes considered in the current study only the first eight terms on the right-hand side of eqn. (8) contribute to the calculations. The last three terms in eqn. (8) pertain to organic compounds having amino- and hydroxyl-functional groups. Results of our $\Delta H_{vap,298K}$ predictions are reported in the second column of Table 5.

Table 5. Comparison of the Enthalpies of Vaporization, $\Delta H_{vap,298K}$ (kJ mol^{-1}), Predicted by the Abraham Model, eqn. (8), and the Group-Additivity Method of Naef and Acree, eqn. (10).

Compound	$\Delta H_{vap,298K}$ **Eqn. (8)**	$\Delta H_{vap,298K}$ **Eqn. (10)**
Hept-2-yne	39.93	40.23
Hept-3-yne	38.66	40.23
Oct-3-yne	43.74	44.81
Non-2-yne	49.81	49.39
Non-3-yne	48.63	49.39
Non-4-yne	48.37	49.39
Dec-2-yne	54.80	53.97
Dec-3-yne	53.54	53.97
Dec-4-yne	53.18	53.97
Dec-5-yne	53.30	53.97
Undec-1-yne	57.57	56.52
Undec-2-yne	59.73	58.55
Undec-3-yne	58.45	58.55
Undec-4-yne	58.07	58.55
Undec-5-yne	58.07	58.55
Dodec-2-yne	64.69	63.12
Dodec-3-yne	63.37	63.12
Dodec-4-yne	62.97	63.12
Dodec-5-yne	62.89	63.12
Dodec-6-yne	62.83	63.12
Tridec-1-yne	66.71	65.68
Tridec-2-yne	69.29	67.71
Tridec-3-yne	67.62	67.71
Tridec-4-yne	67.20	67.71
Tridec-5-yne	57.13	67.71
Tridec-6-yne	66.99	67.71
Tetradec-1-yne	71.34	70.26
Tetradec-2-yne	74.16	72.29
Tetradec-3-yne	72.44	72.29
Tetradec-4-yne	72.05	72.29
Tetradec-5-yne	71.91	72.29
Tetradec-6-yne	71.78	72.29
Tetradec-7-yne	71.74	72.29

We were unable to find experimental $\Delta H_{vap,298K}$ data in the published chemical literature to compare our calculated values against. What we offer in the way of a comparison is to compare our calculated values against the calculated values of a popular group-additivity method proposed by Naef and Acree[62] that has been shown to predict $\Delta H_{vap,298K}$ values for a wide range of organic and organometallic compounds to within a standard deviation of SD = 4.30 kJ mol^{-1} for 3,460 compounds. The basic method sums the contributions that each atomic group makes to the given thermodynamic or physical property:

$$\text{Property} = \sum_i A_i a_i + \sum_j B_j b_j + \text{constant} \qquad (9)$$

where A_i is the number of occurrences of the ith atom group, B_j is the number of times each special group occurs, a_i and b_j are the numerical values of each atom group and special group, and C is a constant.

The atom group-additivity method, proposed by Naef and Acree,[62] fragments linear alkyne molecules into two types of sp hybridized carbon atoms and two types of sp^3 hybridized carbon atoms. Each carbon atom type is based on the number of each type of atoms bonded to the carbon atom. One of the so carbon atom-groups will be bonded to one hydrogen atom (HC#) and the second carbon atom type will be bonded to zero hydrogen atoms (CC#). The symbol "#" was used by Naef and Acree to denote a carbon-carbon atom triple bond. In the case of the sp^3 hybridized carbon atoms one carbon atom is bonded to three hydrogen atoms and one carbon atom (CH_3 group), and the second carbon atom type is bonded to two hydrogen atoms and two carbon atoms (CH_2 group). There is also one special group that is defined as the number of carbon atoms in the unsaturated hydrocarbon molecule.

In eqn. (10) below we have filled in the numerical group values and constants for predicting $\Delta H_{vap,298K}$ of linear alkynes:

$$\Delta H_{vap,298K}\ (\text{kJ mol}^{-1}) = 3.07\, n_{CH3} + 4.67\, n_{CH2} + 2.42\, n_{HC\#} + 6.05\, n_{CC\#} - 0.09\, n_{\text{carbon unsat}} + 8.61 \qquad (10)$$

Examination of the numerical entries in the last two columns of Table 5 reveals that the predictions based on the Abraham model are similar to predictions based on the group-additivity model of Naef and Acree.[61] Except for the 1-alkynes the group-additivity method though is not able to distinguish between the placement of the triple bond in the molecule, and gives the same predicted values for a given molecular formula. In other words, the predicted values of all 2-tetradecyne through 7-tetradecyne molecules are the same. The group additivity model also does not distinguish between "*cis*" and '*trans*" isomers. This limitation is a common feature of most group-additivity and group contribution methods. The Abraham model, on the other hand, would provide different predicted values for the different alkyne isomers, and does not require fragmentation of the molecule into atom groups or functional groups. Fragmentation of molecules into functional groups can be difficult at times, particularly in the case of more complex molecules having many different functional groups.

CONCLUSION

Numerical values of the Abraham model **L** solute descriptor have been reported for the first time for 33 linear C_7-C_{14} alkynes. The numerical values were determined by regression analysis of published isothermal gas chromatographic retention indices on squalane and apiezon L stationary phases. Calculated **L** solute descriptors completed our set of solute descriptors for linear C_7-C_{14} alkynes. Prior to this study our private database of descriptor values contained only the **E**, **S**, **A**, **B** and **V** solute descriptors for these 33 alkyne molecules. Solute descriptors were used to predict the standard molar enthalpies of vaporization based on a previously published Abraham model correlation.[42] The predicted values compare very favourably with calculated values based on an atom-group additivity model.[62] Unlike the additivity model the Abraham model provides different predicted values of $\Delta H_{vap,298K}$ for each linear alkyne isomer that structurally differ from each other by the placement of the triple bond in the molecule.

REFERENCES

[1]Abraham, M. H., Acree, W. E. Jr., Gas-solvent and water-solvent partition of trans-stilbene at 298 K, *J. Mol. Liq*., **2017**, 238, 58-61. https://doi.org/10.1016/j.molliq.2017.04.119

[2]Abraham, M. H. Acree, W. E. Jr., Descriptors for the prediction of partition coefficients of 8-hydroxyquinoline and its derivatives, *Sep. Sci. Technol*., **2014**, *49*, 2135-2141. https://doi.org/10.1080/01496395.2014.928768

[3]Hart, E., Klein, A., Barrera, M., Jodray, M., Rodriguez, K., Acree, W. E. Jr., Abraham, M. H., Development of Abraham model correlations for describing the transfer of molecular solutes into propanenitrile and butanenitrile from water and from the gas phase, *Phys. Chem. Liq*., **2018**, *56*, 821-833. https://doi.org/10.1080/00319104.2017.1399268

[4]Fischer R., Jodray, M., Qian, E., Wang, L., Lee, G., Yue, D., Che, M., Liu, Y., Acree, W. E. Jr., Abraham, M. H., Abraham model correlations for solute transfer into benzyl alcohol from both water and the gas phase, *Phys. Chem. Liq*., **2020**, *58*, 116-126. https://doi.org/10.1080/00319104.2018.1550778

[5]Rabhi, F., Mutelet, F., Sifaoui, H., Wagle, D. V., Baker, G. A., Churchill, B., Acree, W. E. Jr., Characterization of the solubilizing ability of tetraalkylammonium ionic liquids containing a pendant alkyl chain bearing a basic N,N-dimethylamino or N,N-dimethylaminoethoxy functionality, *J. Mol. Liq*., **2019**, *283*, 380-390. https://doi.org/10.1016/j.molliq.2019.03.066

[6]Mutelet, F., Baker, G. A., Ravula, S., Qian, E., Wang, L., Acree, W. E. Jr., Infinite dilution activity coefficients and gas-to-liquid partition coefficients of organic solutes dissolved in 1-sec-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)-imide and in 1-tert-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide, *Phys. Chem. Liq*., **2019**, *57*, 453-472.https://doi.org/10.1080/00319104.2018.1491045

[7]Mutelet, F., Ravula, S., Baker, G. A., Woods, D., Tong, X., Acree, W. E. Jr., Infinite dilution activity coefficients and gas-to-liquid partition coefficients of organic solutes dissolved in 1-benzylpyridinium bis(trifluoromethylsulfonyl)imide and 1-cyclohexylmethyl-1-methylpyrrolidinium bis(trifluoro-methylsulfonyl)imide, *J. Solut. Chem*., **2018**, *47*, 308-335. https://doi.org/10.1007/s10953-018-0720-5

[8]Abraham, M. H., Ibrahim, A., Acree, W. E. Jr., Air to brain, blood to brain and plasma to brain distribution of volatile organic compounds: linear free energy analyses, *Eur. J. Med. Chem*., **2006**, *41*, 494-502. https://doi.org/10.1016/j.ejmech.2006.01.004

[9]Abraham, M. H., Ibrahim, A., Acree W. E. Jr. Air to muscle and blood/plasma to muscle distribution of volatile organic compounds and drugs: linear free energy analyses. *Chem. Res. Toxicol*., **2006**, *19*, 801-808. https://doi.org/10.1021/tx050337k

[10]Abraham, M. H., Ibrahim, A., Acree, W. E., Air to liver partition coefficients for volatile organic compounds and blood to liver partition coefficients for volatile organic compounds and drugs, *Eur. J. Med. Chem*., **2007**, *42*, 743751. https://doi.org/10.1016/j.ejmech.2006.12.011

[11]Abraham, M. H., Ibrahim, A., Acree, W. E., Air to lung partition coefficients for volatile organic compounds and blood to lung partition coefficients for volatile organic compounds and drugs, *Eur. J. Med. Chem*., **2008**, *43*, 478485. https://doi.org/10.1016/j.ejmech.2007.04.002

[12]Abraham, M. H., Ibrahim, A., Air to fat and blood to fat distribution of volatile organic compounds and drugs: Linear free energy analyses. *Eur. J. Med. Chem*., **2006**; *41*: 14301438. https://doi.org/10.1016/j.ejmech.2006.07.012

[13]Hoover, K. R., Acree, W. E. Jr., Abraham, M. H., Chemical toxicity correlations for several fish species based on the Abraham solvation parameter model, *Chem. Res. Toxicol*., **2005**, *18*, 1497-505. https://doi.org/10.1021/tx050164z

[14]Hoover, K. R., Flanagan, K. B., Acree, W. E. Jr., Abraham, M. H. Chemical toxicity correlations for several protozoas, bacteria, and water fleas based on the Abraham solvation parameter model, *J. Environ. Eng. Sci*., **2007**, *6*, 165-174. https://doi.org/10.1139/s06-041

[15]Bowen, K. R., Flanagan, K. B., Acree, W. E., Abraham, M. H., Rafols, C., Correlation of the toxicity of organic compounds to tadpoles using the Abraham model, *Sci. Total Environ*., **2006**, *371*, 99-109. https://doi.org/10.1016/j.scitotenv.2006.08.030

[16]Bowen, K. R., Flanagan, K. B., Acree, W. E., Abraham, M. H., Correlating toxicities of organic compounds to select protozoa using the Abraham model, *Sci. Total Environ*., **2006**, *369*, 109-118. https://doi.org/10.1016/j.scitotenv.2006.05.008

[17]Lu, J. Z, Acree, W. E. Jr., Abraham, M. H., Abraham model correlations for enthalpies of solvation of organic solutes dissolved in N,N-dimethylacetamide, 2-butanone and tetrahydrofuran (UPATED) at 298.15 K, *Phys. Chem. Liq*., **2020**, *58*, 675-692. https://doi.org/10.1080/00319104.2019.1633528

[18]Lu, J. Z., Acree, W. E. Jr., Abraham, M. H., Abraham model correlations for enthalpies of solvation of organic solutes dissolved in methyl acetate and octane, *Phys. Chem. Liq*., **2020**, *58*, 18-30. https://doi.org/10.1080/00319104.2018.1534234

[19]Lu, J. Z., Acree, W. E Jr., Abraham, M. H., Updated Abraham model correlations for enthalpies of solvation of organic solutes dissolved in benzene and acetonitrile, *Phys. Chem. Liq*., **2019**, *57*, 84-99. https://doi.org/10.1080/00319104.2018.1423565

[20]Higgins, E., Acree, W. E. Jr., Abraham, M. H., Development of Abraham model correlations for enthalpies of solvation of organic solutes dissolved in 1,3-dioxolane, *Phys. Chem. Liq*., **2016**, *54*, 786-796. https://doi.org/10.1080/00319104.2016.1161043

[21]Schmidt, A., Zad, M., Acree, W. E. Jr., Abraham M. H., Development of Abraham model correlations for predicting enthalpies of solvation of nonionic solutes dissolved in formamide, *Phys. Chem. Liq*., **2016**, *54*: 313-324. https://doi.org/10.1080/00319104.2015.1084882

[22]Hart, E., Grover, D., Zettl, H., Koshevarova, V., Acree, W. E. Jr., Abraham M. H., Development of Abraham model expressions for predicting the enthalpies of solvation of solutes dissolved in acetic acid, *Phys. Chem. Liq*., ***2016***, *54*, 141-154. https://doi.org/10.1080/00319104.2015.1079194

[23]Hart, E., Grover, D., Zettl, H., Acree, W. E. Jr., Abraham, M. H., Abraham model enthalpy of solvation correlations for solutes

dissolved in dimethyl carbonate and diethyl carbonate, *Phys. Chem. Liq.*, 2015, 53, 732-747. https://doi.org/10.1080/00319104.2015.1042478

[24]Hart, E., Zettl, H., Grover, D., Acree, W. E. Jr., Abraham, M. H., Abraham model enthalpy of solvation correlations for solutes dissolved in 1-alkanol solvents (C4-C6), *Phys. Chem. Liq*., **2015**, *53*, 638-659. https://doi.org/10.1080/00319104.2015.1018259

[25]Mintz, C., Clark, M., Burton, K., Acree, W. E. Jr., Abraham, M. H., Enthalpy of solvation correlations for gaseous solutes dissolved in benzene and in alkane solvents based on the Abraham model, *QSAR Comb. Sci*., **2007**, *26*, 881-888. https://doi.org/10.1002/qsar.200630152

[26]Mintz, C., Burton, K., Acree, W. E. Jr., Abraham, M. H., Enthalpy of solvation correlations for gaseous solutes dissolved in linear alkanes (C_5-C_{16}) based on the Abraham model, *QSAR Comb. Sci*., **2008**, *27*, 179-186. https://doi.org/10.1002/qsar.200730040

[27]Mintz, C., Burton, K., Ladlie, T., Clark, M., Acree, W. E. Jr., Abraham, M. H., Enthalpy of solvation correlations for organic solutes and gases dissolved in N,N-dimethylformamide and tert-butanol, *J. Mol. Liq.*, **2009**, *144*, 23-31. https://doi.org/10.1016/j.molliq.2008.09.002

[28]Abraham, M. H. Acree, W. E. Jr., Descriptors for the α,ω-dicarboxylic acids from oxalic acid to sebacic acid, *Fluid Phase Equilib*., **2018**, *467*, 17-24. https://doi.org/10.1016/j.fluid.2018.03.017.0378-3812

[29]Acree, W. E. Jr., Jodray, M., Abraham, M. H., Illustration of the calculation of solute descriptors for maltol from published solubility data, *Phys. Chem. Liq*., **2018**, *56*, 403-409. https://doi.org/10.1080/00319104.2017.1376061

[30]Acree W. E. Jr., Bowen, K. R., Horton, M. Y., Abraham, M. H., Computation of Abraham model solute descriptors for 3-methyl-4-nitrobenzoic acid from measured solubility data, *Phys. Chem. Liq*., **2017**, *55*, 482-491. https://doi.org/10.1080/00319104.2016.1227813

[31]Abraham, M. H., Acree, W. E. Jr., Brumfield, M., Hart, E., Pipersburgh, L., Mateja, K., Dai, C., Grover, D., Zhang, S., Deduction of physicochemical properties from solubilities: 2,4-dihydroxy-benzophenone, biotin, and caprolactam as examples, *J. Chem, Eng. Data*, **2015**, *60*, 1440-1446. https://doi.org/10.1021/je501140p

[32]Abraham, M. H., Gola, J. M. R., Cometto-Muniz, J. E., Cain, W. S., The correlation and prediction of VOC thresholds for nasal pungency, eye irritation and odour in humans, *Indoor+Built Environ*., **2001**, *10*, 252-257. https://doi.org/10.1177/1420326X0101000320

[33]Abraham, M. H., Hassanisadi, M., Jalali-Heravi, M., Ghafourian, T., Cain, W. S., Cometto-Muniz, J. E., Draize rabbit eye test compatibility with eye irritation thresholds in humans: A quantitative structure-activity relationship analysis, *Toxicol. Sci*., **2003**, *76*, 384-391.

https://doi.org/10.1093/toxsci/kfg242

[34]Abraham, M. H., Kumarsingh, R., Cometto-Muniz, J. E., Cain, W. S., Draize eye scores and eye irritation thresholds in man can be combined into one QSAR, *Ann. New York Acad. Sci*., **1998**, *855*, 652-656. https://doi.org/10.1111/j.17496632.1998.tb10641.x

[35]Cometto-Muniz, J. E., Cain, W. S., Abraham, M. H., Determinants for nasal trigeminal detection of volatile organic compounds, *Chem. Senses*, **2005**, *30*, 627-642. https://doi.org/10.1093/chemse/bji056

[36]Abraham, M. H., Kumarsingh, R., Cometto-Muniz, J. E., Cain, W. S., An algorithm for nasal pungency thresholds in man, *Arch. Toxicol*., **1998**, *72*, 227-232. https://doi.org/10.1007/s002040050493

[37]Abraham, M. H., Andonian-Haftvan, J., Cometto-Muniz, J. E., Cain, W. S., An analysis of nasal irritation thresholds using a new solvation equation, *Fund. Appl. Toxicol.*, **1996**, *31*, 71-76. https://doi.org/10.1006/faat.1996.0077

[38]Abraham, M. H., Martins, F., Human skin permeation and partition: general linear free-energy relationship analyses, *J. Pharm. Sci*., **2004**, *93*, 1508-1523. https://doi.org/10.1002/jps.20070

[39]Zhang, K., Abraham, M. H., Liu, X., An equation for the prediction of human skin permeability of neutral molecules, ions and ionic species, *Int. J. Pharm*., **2017**, *521*, 259-266. https://doi.org/10.1016/j.ijpharm.2017.02.059

[40]Abraham, M. H., Acree, W. E. Jr., Mintz, C., Payne, S., Effect of anesthetic structure on inhalation anesthesia: implications for the mechanism, *J. Pharm. Sci*., **2008**, *97*, 2373-2384. https://doi.org/10.1002/jps.21150

[41]Abraham, M. H., Acree, W. E Jr., Prediction of convulsant activity of gases and vapors, *Eur. J. Med. Chem*., **2009**, *44*, 885-890. https://doi.org/10.1016/j.ejmech.2008.05.027

[42]Churchill, B., Acree, W. E. Jr., Abraham, M. H., Development of Abraham model expressions for predicting the standard molar enthalpies of vaporization of organic compounds at 298.15 K, *Thermochim. Acta*, **2019**, *681*, 178372/1-178372/6. https://doi.org/10.1016/j.tca.2019.178372

[43]Abraham, M. H., Acree, W. E. Jr., Estimation of enthalpies of sublimation of organic, organometallic and inorganic compounds, *Fluid Phase Equilib*., **2020**, *515*, 112575/1-112475/5. https://doi.org/10.1016/j.fluid.2020.112575

[44]Abraham, M. H., Acree, W. E. Jr., Estimation of vapor pressures of liquid and solid organic and organometallic compounds at 298.15 K, *Fluid Phase Equilib*., **2020**, *519*, 112595/1-112595/5. https://doi.org/10.1016/j.fluid.2020.112595

[45]Abraham, M. H., Acree, W. E., Estimation of heat capacities of gases, liquids and solids, and heat capacities of vaporization and of sublimation of organic chemicals at 298.15 K, J. Mol. Liq., **2020**, 317, 113969/1-113969/4. https://doi.org/10.1016/j.molliq.2020.113969

[46]Abraham, M. H., Acree, W. E. Jr., Descriptors for artemisinin and its derivatives; estimation of physicochemical and biochemical data, *Eur. Chem. Bull*., **2013**, *2*, 1027-1037. http://dx.doi.org/10.17628/ecb.2013.2.1027-10

[47]Bowen, K. R., Stephens, T. W., Lu, H., Satish, K., Shan, D., Acree, W. E. Jr., Abraham, M. H., Experimental and predicted solubilities of 3,4-dimethoxybenzoic acid in select organic solvents of varying polarity and hydrogen-bonding character, *Eur. Chem. Bull*., **2013**, *2*, 577-583. http://dx.doi.org/10.17628/ecb.2013.2.577-58

[48]Wilson, A., Tian, A., Chou, V., Quay, A. N., Acree, W. E. Jr., Abraham, M. H., Experimental and predicted solubilities of 3,4-dichlorobenzoic acid in select organic solvents and in binary aqueous-ethanol mixtures, *Phys. Chem. Liq*., **2012**, *50*, 324-335. https://doi.org/10.1080/00319104.2012.673166

[49]Poole, C. F., Ariyasena, T. C., Lenca, N., Estimation of the environmental properties of compounds from chromatographic properties and the solvation parameter method. *J. Chromatogr. A.*, **2013**, *1317*, 85-104. https://doi.org/10.1016/j.chroma.2013.05.045

[50]Clarke, E. D., Mallon, L., The Determination of Abraham descriptors and their Application to Crop Protection Research, in *Modern Methods in Crop Protection Research*, ed. Jeschke, P., Krämer, W., Schirmer, E., Witschel, M., Wiley-VCH Verlag GmbH & Co., **2012**.

[51]Endo, S., Goss, K.-U., Applications of polyparameter linear free energy relationships in environmental chemistry, *Environ. Sci. Technol*., **2014**, *48*, 12477-12491. https://doi.org/10.1021/es503369t

[52]Jalan, A., Ashcraft, R. W., West, R. H., Green, W. H., Predicting solvation energies for kinetic modeling, *Ann. Rep. Prog. Chem, Sect. C: Phys. Chem*., **2010**, *106*, 211-258. https://doi.org/10.1039/B811056P

[53]Abraham, M. H., Acree, W. E. Jr., Liu, X., Descriptors for high-energy nitro compounds; Estimation of thermodynamic, physiochemical and environmental properties, *Prop. Explos. Pyrotech*., in press. https://doi.org/10.1002/prep.202000117

[54]Abraham, M H., Acree, W. E. Jr., Liu, X., Descriptors for adamantane and some of its derivatives, *J. Mol. Liq*., *submitted for publication.*

[55]Liu, G., Eddula, S., Jiang, C., Huang, J., Tirumala, P., Xu, A., Acree, W. E. Jr., Abraham, M. H., Abraham solvation parameter model: prediction of enthalpies of vaporization and sublimation of mono-methyl branched alkanes using measured gas chromatographic data, *Eur. Chem. Bull*., **2020**, 9, 273-284. http://dx.doi.org/10.17628/ecb.2020.9.273-284

[56]Tirumala, P., Huang, J., Eddula, S., Hiang, C., Xu, A., Liu, G., Acree, W. E. Jr., Abraham, M. H., Calculation of Abraham model L-descriptor and standard molar enthalpies of vaporization and sublimation for C9 - C26 mono-alkyl and polymethyl alkanes, *Eur. Chem. Bull*., **2020**, *9*, 317-328. http://dx.doi.org/10.17628/ecb.2020.9.317-328

[57]Ulrich N., Endo S., Brown T. N., Watanabe N., Bronner G., Abraham M. H., Goss K-U., UFZ-LSER database v 3.2.1 [Internet], Leipzig, Germany, Helmholtz Centre for Environmental Research-UFZ. 2017 [accessed on 27.10.2020]. Available from http://www.ufz.de/lserd.

[58]Rang, S., Kuningas, K., Orav, A., Eisen, O., Capillary gas chromatography of n-alkynes. I. Retention indices, *J. Chromatog.*, **1976**, *119*, 451-460. https://doi.org/10.1016/S0021-9673(00)86807-7

[59]Sojak, L., Hrivnak, J., Majer, P., Capillary gas chromatography of linear alkenes on squalane, *Anal. Chem*., **1973**, *45*, 293-302. https://doi.org/10.1021/ac60324a039

[60]Vigdergauz, M. S., Nasybullina, R. K., Polyakova, L. A, Byl'ev, V. A., Methods of assessing fuel and oil quality: The use of apiezons as stationary phases in gas chromatography, *Khim. Tekhnol. Topliv Masel*, **1968**, *11*, 57-61.

[61]Sojak, L., Krupcik, J., Janak, J., Gas chromatography of all C15-C18 linear alkenes on capillary columns with very high resolution power, *J. Chromatog*., **1980**, *195*, 43-64. https://doi.org/10.1016/S0021-9673(00)81542-3

[62]Naef, R., Acree, W. E., Jr., Calculation of five thermodynamic molecular descriptors by means of a general computer algorithm based on the group-additivity method: standard enthalpies of vaporization, sublimation and solvation, and entropy of fusion of ordinary organic molecules and total phase-change entropy of liquid crystals, *Molecules*, **2017**, *22*, 1059/1-1059/41. https://doi.org/10.3390/molecules22071059

Received: 04.12.2020.
Accepted: 25.12.2020.