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Reliable method for prediction of the flash point of various classes of amines on the basis of some molecular moieties for safety measures in industrial processes

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ABSTRACT

This work presents a novel, reliable and simple method of estimating the flash point of various types of flammable amines, which are important for safety measures in industrial processes. Different amines include aliphatic amines such as primary, secondary, tertiary and cyclic amines as well as aromatic amines and hetero arenes containing nitrogen heteroatom. The proposed correlation is based on the contribution of some specific molecular moieties and functional groups, which can easily be used for any types of amines. Intermolecular forces are important in the new method, which are counted by two increasing and decreasing parameters. The root mean square (rms) deviation is 18 K for different classes of amines including 133 diverse compounds. The estimated flash points have been compared with one of the best available predictive methods, which gives much lower value of the rms deviation.

1. Introduction

The flash point is the lowest temperature at which the mixture of vapor and air above the surface of the liquid can be ignited. It is frequently used to characterize the flammability of combustible liquids and solids. Since accurate knowledge of flash point is essential to asses the fire hazard associated with designing process, transportation and storage systems, reliable methods for prediction of different classes of organic compounds are utmost important. Moreover, there are many important chemicals or new synthesized compounds for which no flash point data are given. Since some classes of organic compounds have dangerous properties such as: (a) sensitivity to impact (Keshavarz, 2010a), electric spark (Keshavarz, Motamedoshariati, Pouretedal, Kavosh Tehrani, & Semnani, 2007), shock (Keshavarz, 2011a) and heat (Keshavarz, 2011b) for high explosives; (b) flammability of their vapors with air (Agrawal, 2010; Keshavarz, 2003/2006; Keshavarz, Ramadan, Mousaviazar, Zali, Esmailpour et al., 2011; Keshavarz, Ramadan, Mousaviazar, Zali, & Shokrollahi, 2011) and (c) toxicity of vapors (Pouretedal and Keshavarz, 2011), the measurements of flash points are more difficult for these compounds.

Since the flash point is related to volatility and thermodynamic properties, the majority of predictive methods require accurate values of thermodynamic properties, typically vapor pressure, boiling point and enthalpy of vaporization (Bagheri, Bagheri, Heidari, & Fazeli, 2012; Gharagheizi, Keshavarz, & Sattari, 2012; Kim & Lee, 2010; Liu & Liu, 2010; Rowley, Freeman et al., 2010; Valenzuela, Vázquez-Román, Patel, & Mannan, 2011). However, the experimental data of required thermodynamic properties or reliable estimated methods for phase transitions such as heats of sublimation (Keshavarz, 2008, 2010b; Keshavarz & Yousefi, 2008) may be needed in these methods. The other widely used approaches consist of neural networks and methods of estimating properties based on structural contributions. Although different methods on the basis of neural networks can be used for wide range of organic compounds through training and test sets, they are not widely implemented because: (a) they depend on specialized software, such as Dragon (Todeschini, Consonni, & Pavan, 2002), and quantitative structure–property relationships (QSPR); (b) they often require unusual molecular descriptors through specialized software; (c) the compounds with similar molecular structure in training set of the QSPR procedure should be used as test set. Meanwhile, there is no need to use specialized software for prediction of flash point based on structural contributions. For general

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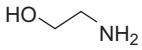
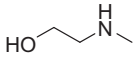
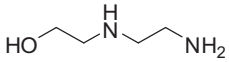
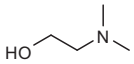
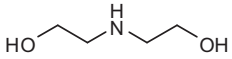
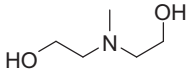
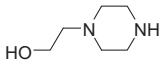
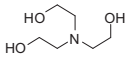
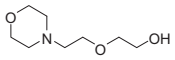
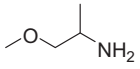
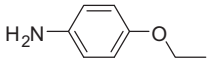
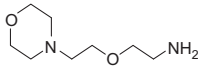
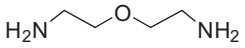
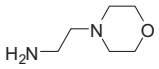
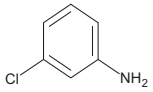
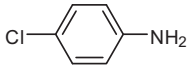
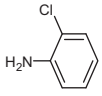
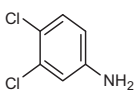
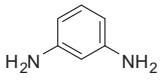
Table 1
Comparison of the predicted flash points of Eq. (2) and Eq. (1) as well as group contribution method of Rowley, Rowley et al. (2010) with experimental data (Project 801, 2006).

No.	Compound	Molecular formula	Exp.	Eq. (1)	Dev.	Eq. (2)	Dev.	Rowley et al.	Dev.
1		C_2H_7NO	358	273	−85	317	−41	342	−16
2		C_3H_9NO	345	281	−64	325	−20	336	−9
3		$C_4H_{11}NO$	318	288	−30	334	16	315	−3
4		$C_4H_{12}N_2O$	375	331	−44	376	1	384	9
5		$C_4H_{11}NO$	314	288	−26	334	20	315	1
6		$C_4H_{11}NO_2$	425	288	−137	399	−26	433	8
7		$C_5H_{13}NO_2$	400	296	−104	408	8	409	9
8		$C_6H_{15}NO$	321	303	−18	352	30	332	11
9		$C_6H_{14}N_2O$	397	356	−41	408	11	393	−4
10		$C_6H_{15}NO_3$	453	303	−150	481	28	498	45
11		$C_8H_{17}NO_3$	403	329	−74	403	0	441	38
12		$C_4H_{11}NO$	281	288	7	289	8	285	4
13		$C_8H_{11}NO$	389	362	−27	382	−7	370	−19
14		$C_8H_8N_2O_2$	388	372	−16	380	−8	402	14
15		$C_4H_{12}N_2O$	360	331	−29	331	−29	346	−14
16		$C_6H_{14}N_2O$	359	356	−3	344	−16	361	2
17		C_6H_6NCl	378	352	−26	379	1	376	−2
18		C_6H_6NCl	386	352	−34	379	−7	376	−10
19		C_6H_6NCl	364	352	−12	379	15	376	12
20		$C_6H_5NCl_2$	439	357	−82	412	−27	434	−5
21		$C_6H_8N_2$	411	389	−22	414	2	371	−40

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