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## Thermochemical stability: A comparison between experimental and predicted data

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## ABSTRACT

The first step to be performed during the development of a new industrial process should be the assessment of all hazards associated to the involved compounds. Particularly, the knowledge of all substances thermochemical parameters is a primary feature for such a hazard evaluation. CHETAH (CHEMical Thermodynamic And Hazard evaluation) is a prediction software suitable for calculating potential hazards of chemicals, mixtures or a single reaction that, using only the structure of the involved molecules and Benson's group contribution method, is able to calculate heats of formation, entropies, Gibbs free energies and reaction enthalpies. Because of its ability to predict the potential hazards of a material or mixture, CHETAH is part of the so-called "desktop methods" for early stage chemical safety analysis.

In this work, CHETAH software has been used to compile a complete risk database reporting heats of decomposition and Energy Release Potential (ERP) for 342 common use chemicals. These compounds have been gathered into classes depending on their functional groups and similarities in their thermal behavior. Calculated decomposition enthalpies for each of the compounds have also been compared with experimental data obtained with either thermoanalytic or calorimetric techniques (Differential Scanning Calorimeter – DSC – and Accelerating Rate Calorimeter – ARC).

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### 1. Introduction

Systematic search for hazards, risk assessment and identification of possible remedies are the basic steps of risk analysis (Stoessel, 2008). Chemical industry, more than any others, is perceived as a potential threat for mankind and environment. Nevertheless, all the benefits arising from its activities cannot be disregarded: drugs for human health, crop protection, new materials, colors, textiles and so on. One of the reasons contributing to this negative perception is the occurrence of major accidents, such as those ones which took place in Seveso and Bhopal, that, even if are rare, unavoidably retain public attention. Therefore, in order to minimize and, if possible, eliminate such catastrophic events, a number of studies about the chemical risk associated to the thermal stability of compounds or reacting mixtures has been carried out throughout the last 35 years (Barontini, Cozzani, & Petarca, 2001; Cardillo, 2001; Cardillo & Cattaneo, 1991; Cardillo, Gigante, Lunghi,

Fraleoni Morgera, & Zanirato, 2008; Cardillo, Gigante, Lunghi, & Zanirato, 2010; Cardillo & Girelli, 1980; Copelli et al., 2011a, 2011b; Di Somma et al., 2010; Dien, Fierz, Stoessel, & Kille, 1994; Fayet, Rotureau, Joubert, & Adamo, 2011; Frurip et al., 1995; Lunghi et al., 2004; Maestri et al., 2009; Roduit et al., 2005; Sato & Sugawara, 1985; Sempere, Nomen, Serra, & Cardillo, 1997).

Chemical risk associated with thermally unstable materials or systems is sometimes predictable from both complete thermodynamic knowledge and correct interpretations of the fundamental laws of physical chemistry. The first step in the identification of thermal dangers consists in evaluating the thermodynamic potential of the system: that is, determining whether the reaction is thermodynamically favored and, subsequently, how much thermal energy releases. The amount of heat evolved can be related to the adiabatic temperature rise and, then, to the instability of reactants, products or reaction mass. Therefore, if it is possible to know or calculate in advance all the thermal effects of an undesired reaction, it is possible, at least as a first approximation, to predict the hazard.

Basing on these features, it is very important to possess suitable tools aimed to determine the thermodynamic potential associated to a chemical compound or a mixture with a quite high level of

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reliability. Particularly, such a fundamental property can be estimated both theoretically, through the use of dedicated evaluation software, and experimentally, performing suitable thermoanalytic and calorimetric tests.

Aim of this work has been the compilation of a complete chemical risk database, capable of constituting an easy tool to be consulted in order to obtain preliminary information about potential hazards associated with a certain compound that needs to be handling for a variety of reasons. Particularly, CHETAH software has been used to compile such a database by reporting heats of decomposition and Energy Release Potential (ERP) for 342 common use chemicals. These compounds have been gathered into classes depending on their functional groups and similarities in their thermal behavior.

In order to validate CHETAH theoretical predictions, calculated decomposition enthalpies for each of the compounds have been compared with experimental data obtained with either thermoanalytic or calorimetric techniques (Differential Scanning Calorimeter – DSC – and Accelerating Rate Calorimeter – ARC).

## 2. Software and laboratory instruments

### 2.1. CHETAH software

An important tool for the theoretical computation of chemical risk is CHETAH (CHEMical Thermodynamic And Hazard evaluation) software, that it was first presented in 1974 (Seaton, Freedman, & Treweek, 1974) and now it is commercialized by ASTM (Harrison, Madas, & Sharma, 2005).

Because of its ability to predict the hazards of a substance or a mixture only by the knowledge of the chemical structure, CHETAH is ideal for a preliminary assessment, performing various calculations such as: (1) estimation of reaction heats; (2) estimation of thermodynamic properties of individual substances; (3) prediction of the tendency of a compound or a mixture to propagate a deflagration or a detonation.

Heats of formation, entropies and free energies of the substances in question are calculated using the Benson's criterion (Benson, 1976).

The estimation of the hazard associated to a substance is formulated on the basis of four criteria.

The first criterion consists in the calculation of the maximum amount of energy released during a decomposition event (maximum heat of decomposition,  $\Delta\hat{H}_{\text{dec, max}}$ ). In order to perform such a calculation, the software assumes that, when a generic compound of formula  $C_xH_yO_zN_k$  decomposes, the obtained products are:  $\text{CO}_2$ ,  $\text{H}_2\text{O}$ ,  $\text{N}_2$ ,  $\text{CH}_4$ ,  $\text{C}$ ,  $\text{H}_2$  and  $\text{O}_2$ . Then, the software calculates the combination of these products that maximizes the heat of decomposition. As the sake of example, if the decomposition of pure water is considered, the set of products that maximizes the heat of decomposition (calculated basing on Benson's groups additive method) is:  $\text{H}_2$  and  $\text{O}_2$ . CHETAH considers the risk as low, medium or high depending on the value assumed by such a maximum heat of decomposition (see Table 1). In a similar way, that is assuming complete combustion ( $\text{CO}_2$  and  $\text{H}_2\text{O}$  as final products), the maximum heat of combustion,  $\Delta\hat{H}_{\text{comb, max}}$ , is evaluated.

**Table 1**  
First CHETAH criterion for chemical risk evaluation.

High level risk	$\Delta\hat{H}_{\text{dec, max}} < -0.7 \text{ kcal/g}$
Medium level risk	$-0.7 \text{ kcal/g} < \Delta\hat{H}_{\text{dec, max}} < -0.3 \text{ kcal/g}$
Low level risk	$\Delta\hat{H}_{\text{dec, max}} > -0.3 \text{ kcal/g}$

**Table 2**  
Third CHETAH criterion for chemical risk evaluation.

High level risk	$-80 < B_0 < 120$
Medium level risk	$120 < B_0 < 240$ $-160 < B_0 < -80$
Low level risk	$B_0 < 240$ $B_0 < -160$

The second criterion is based on the assumption that the most reactive substances almost always contain many oxygen atoms in their structure; with these materials the difference between the maximum heat of decomposition,  $\Delta\hat{H}_{\text{dec, max}}$ , and the maximum heat of combustion,  $\Delta\hat{H}_{\text{comb, max}}$ , at stoichiometric conditions is small. This means that almost all oxygen required for a complete combustion and/or decomposition is available directly into the analyzed molecule. Therefore, the second criterion is represented by the difference  $\Delta\hat{H}_{\text{comb, max}} - \Delta\hat{H}_{\text{dec, max}}$ . More such a difference tends to zero, the greater the risk is.

The third criterion is based on the concept of "oxygen balance" proposed by Lathrop and Handrix. For a molecule containing  $x$  carbon atoms,  $y$  oxygen atoms and  $z$  hydrogen atoms, the oxygen balance  $B_0$  is obtained by the following formula:

$$B_0 = \frac{1600(2x + y/2 - z)}{\text{PM}} \quad (1)$$

where PM is the molecular weight of the analyzed compound (kg/kmol).

In practice, the oxygen balance defines how much oxygen grams are required to completely oxidize 100 g of compound. More this index is close to zero (that is, all the oxygen required for the full oxidation is already present in the molecule), the more the risk is high (see Table 2). Nevertheless, oxygen balance must be critically assessed; as an example, two isomers with the same value of  $B_0$ , may be, the first, an explosive and, the second, a stable substance: peracetic acid  $\text{CH}_3\text{—CO—O—OH}$  is an explosive while glycolic acid  $\text{HO—CH}_2\text{—COOH}$  is not. In fact, in the calculation of  $B_0$  are counted, without distinction, all the oxygen atoms regardless of the type of linkage in which they are involved. But, as it is well known, the explosive character depends largely on the nature of these links.

The fourth criterion is represented by the following equation:

$$Y = \frac{10 \times \Delta\hat{H}_{\text{dec, max}}^2 W}{n} \quad (2)$$

where  $W$  is the compound weight and  $n$  is the number of atoms in the molecule. Such a formula takes into account both the maximum decomposition enthalpy and the average molecular weight of an atom in the molecule. The square associated to  $\Delta\hat{H}_{\text{dec, max}}$  is merely empirical and it is used to magnify the value of the decomposition enthalpy (especially when it is close to (or major of) 1 kcal/g). Moreover, the higher the average molecular weight of a single compound atom is, the higher the decomposition risk of such a compound will be. The associated risk level is reported in Table 3.

Finally, CHETAH provides a risk value for each of the four criteria and a total risk value, the so-called Energy Release Potential (ERP) (Frurip et al., 1995; Treweek et al., 1978).

**Table 3**  
Forth CHETAH criterion for chemical risk evaluation.

High level risk	$Y > 110$
Medium level risk	$30 < Y < 110$
Low level risk	$Y < 30$

## 2.2. Differential Scanning Calorimeter (DSC)

This calorimetric technique allows for reactants and products thermochemical characterization by comparing the thermal behavior of a sample with that one of a reference. Particularly, sample and reference increase their temperature at a constant fixed rate: whenever a physico-chemical effect occurs in the sample, the heat released (or absorbed) will tend to increase (or decrease) the sample temperature. The result is a temperature difference between sample and reference. The instrument task is to balance such a temperature difference with an appropriate electrical power regulating the reference temperature. The evaluation of this electrical power is a direct measure of the energy due to the transformation that occurs in the sample. In this way, the instrument is able to record the rate at which the sample develops or absorbs heat ( $dQ/dt$ ) during the transformation and to generate characteristic diagrams that report heat power exchanged between sample and reference versus temperature ( $dQ/dt$  vs.  $T$ ) or time ( $dQ/dt$  vs.  $t$ ). These diagrams show the number and the characteristics of all thermal effects, the temperatures (or times) at which these effects take place and, finally, the importance of these ones.

## 2.3. Accelerating Rate Calorimeter (ARC)

ARC, produced by the Columbia Scientific Instruments, is an adiabatic calorimeter controlled by a microprocessor and a data system of analysis particularly suitable to study homogeneous reacting systems subject to decomposition. It is composed of the following items: a spherical sample holder, built of Hastelloy C and placed in an insulated vessel; a radiant heater, which raises sample temperature up to a determined value; a thermocouple connected to the sample holder wall and employed to record sample temperature; an insulated covering (jacket) with three thermocouples and eight heaters (this configuration guarantees to heat the oven up with the same rate as the sample holder during an exothermic reaction); and a capillary tube that links the sample holder to a pressure transducer.

Two different typologies of experiments can be performed by ARC:

- “Iso-aging” test: the instrument keeps the sample in isothermal conditions until an exothermic effect is detected, then the test continues in adiabatic mode.
- Dynamic standard “HEAT”-“WAIT”-“SEARCH” (HWS) test: the sample is warmed up (HEAT) by a radiant heater at a desired temperature, then the instrument waits (WAIT) until all temperatures are stabilized, and, finally, it starts to search for exothermic effects (SEARCH), namely, a self-heating rate of reaction mass into the sample larger than  $0.02$  °C/min. This research terminates when either a predetermined time is passed (15 min) or a sample self-heating rate that exceeds  $0.02$  °C/min is detected. If an exothermic reaction is revealed, the instrument automatically collects temperature and pressure data as functions of time, shifting to adiabatic mode until the reaction ends (self-heating rate lower than the fixed limit). If an exothermic reaction is not revealed, a new sequence of HWS is started at a higher temperature.

From a single ARC test, it is possible to obtain several pieces of information, including initial and end temperature of any detected exothermic effects, sample self-heating rate at any temperature, adiabatic temperature increase, pressure at any temperature and pressure increase rate.

Results obtained are strictly dependent on sample holder thermal inertia  $\Phi$ , which is the ratio of the sum of sample and

sample holder heat capacity with respect to sample heat capacity. Consequently, experimental data have to be corrected to take into account this effect. Temperature and pressure operating ranges between the different test typologies that may be conducted varying from  $25$  to  $500$  °C and from  $1$  to  $170$  bar, respectively.

## 3. Results

Since 1990, the thermochemistry laboratory of Stazione Sperimentale per i Combustibili (Division of Innovhub – SSI) uses CHETAH software as a screening tool just before carrying out each experimental calorimetric test aimed to determine the thermochemical stability of a generic substance (Cardillo, 1998).

In this work, 342 chemical compounds have been evaluated using CHETAH software with the aim of compiling a complete chemical risk database. Particularly, it has been studied their thermal stability behavior.

CHETAH evaluations for each homologous class have been compared with the results arising from both thermoanalytic and calorimetric techniques. In this work, both a Differential Scanning Calorimeter (DSC) and an Accelerating Rate Calorimeter (ARC) have been used to carry out all experimental tests.

Particularly, DSC tests have been run in closed stainless steel crucibles according to ASTM method E 537 using a heating ramp rate of  $5/10$  °C/min (from  $30$  up to  $300$  °C). DSCs have been run first in air (static air remaining in the crucible) and, then, in nitrogen, loading the sample in an inert atmosphere through a special device developed by SSC (Cardillo et al., 1991). In this way it is possible to easily discriminate between thermal effects due to oxidations and thermal effects arising from a decomposition of the analyzed compound.

ARC tests have been run in hastelloy C bombs according to ASTM method E 1981, using a standard Heat-Wait-Search test program between  $30$  °C and  $400$  °C with few grams of sample compound (typically  $2$  or  $3$  g). Atmosphere in the calorimetric bomb is constituted by air but all thermal effects detected can be ascribed to decompositions only because there is not enough contact surface between air and sample to trigger an oxidation.

All the obtained results have been reported in Tables A1–A15 as comparisons between predicted and experimental data. For each compound, heat of formation in the gaseous state ( $\Delta\hat{H}_f$ ), maximum heat of decomposition ( $\Delta\hat{H}_{dec, max}$ , 1st CHETAH criterion), ERP, used instrument (DSC/ARC), detected onset temperature ( $T_{on}$ , if any), experimental heat of decomposition ( $\Delta\hat{H}_{dec}$ , if any) and percentage error of theoretical CHETAH predictions with respect to experimental results ( $\varepsilon = (\Delta\hat{H}_{dec, max} - \Delta\hat{H}_{dec})100/\Delta\hat{H}_{dec, max}$ ), are listed. Particularly, for what concern the computation of the percentage error it is important to observe that, whenever no decomposition event has been detected in the range of operating conditions experimentally tested, such a value has not been computed because it would be irrelevant (always equal to 100%). In the following subsections, a brief summary of the results obtained for each class of compounds is presented, referring to tables reported in the Annex.

Table 4 summarizes, in an easy-to-use format, the comparison between experimental tests and theoretical predictions in terms of observed energy release potential (ERP). One of the most interesting results of this research is that the average percentage of agreement between predicted (CHETAH) and experimental (DSC and ARC) ERP is very high (over 80%) for all classes of compounds apart two: nitriles (46.7%) and heterocyclic compounds (60.4%). In these cases, CHETAH tends to overestimate the decomposition tendency providing a great number of high ERP where no decomposition event can be experimentally detected in the investigated temperatures range. Moreover, it is possible to observe that about 45% of the analyzed compounds show a high risk level, which

**Table 4**  
Summary of the results reported into the chemical risk database.

Class	Number of samples	CHETAH ERP		DSC/ARC exothermic effect		% (ERP results in agreement)
		High	Low	Yes	No	
Nitro compounds	54	52	2	45	9	87.3
Epoxides	9	8	1	8	1	100
Peroxides	5	5	0	5	0	100
Aldehydes	17	9	8	6	11	82.4
Nitriles	16	13	3	5	11	46.7
Acids	29	0	29	0	29	100
Alcohols	10	1	9	1	9	100
Ketones	21	0	21	0	21	100
Hydrocarbons	8	0	8	0	8	100
Heterocyclic compounds	53	33	20	12	41	60.4
Halogen compounds	45	1	44	0	45	97.8
Ethers	4	0	4	0	4	100
Esters	15	1	14	1	14	100
Amines	40	0	40	0	40	100
Amides	15	0	15	0	15	100

means that they are unstable with a strong inclination to exhibit an exothermic decomposition followed by a relief of gaseous products. Analyzing the structural formula of these compounds it is possible to recognize all the main functional groups accounting for such an instable behavior (Bretherick, 1999): nitro compounds, epoxides and peroxides.

Finally, a brief statistical analysis on predicted and experimental decomposition enthalpies has been performed using a method proposed by Fox (1984) and, then, modified by Hanna (1993). Particularly, the following groups need to be calculated: geometric mean (GM) bias, geometric variance (GV) and fraction within a factor of two (FAC2):

$$GM = \exp \left( \text{mean} \left[ \ln \left( \frac{\hat{\Delta H}_{EXP}}{\hat{\Delta H}_{CHETAH}} \right) \right] \right) \quad (3)$$

$$GV = \exp \left[ \text{mean} \left[ \left( \ln \left( \frac{\hat{\Delta H}_{EXP}}{\hat{\Delta H}_{CHETAH}} \right) \right)^2 \right] \right] \quad (4)$$

$$FAC2 = \frac{n_{FAC2}}{n_{TOT}} \quad (5)$$

where  $\hat{\Delta H}_{EXP} = \Delta \hat{H}_{dec}$ ,  $\hat{\Delta H}_{CHETAH} = \Delta \hat{H}_{dec, max}$ ,  $n_{FAC2}$  represents the number of processable data ( $\epsilon \neq 100\%$ ) in a given class of compounds for which the value of the ratio  $\hat{\Delta H}_{EXP}/\hat{\Delta H}_{CHETAH}$  is comprised in between 0.5 and 2;  $n_{TOT}$  represents the total number of processable data for a given class of compounds.

A “perfect” prediction software would have both GM and GV equal to 1.0. Geometric mean bias values of 0.5–2.0 can be thought of as “factor of two” overpredictions and underpredictions in the mean, respectively. A geometric variance value of about 1.6 indicates a typical factor of two scatter between the individual pairs of observed and predicted values. If there is only a mean bias in the predictions and no random scatter is present, then the relation:

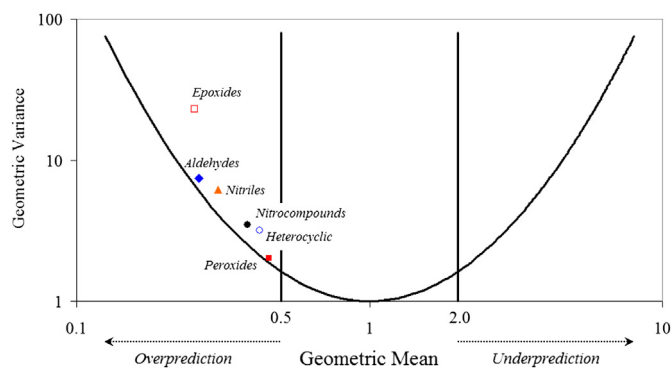
$$\ln GV = (\ln GM)^2 \quad (6)$$

is valid, defining the minimum possible value of GV for a given GM. Parabolic lines representing this relation and vertical lines representing the “factor of two” relation for GM are drawn in Fig. 1, where the results for all the processable functional groups (epoxides, nitro compounds, aldehydes, nitriles, heterocyclic compounds and

peroxides) have also been reported. All data must be compulsory comprised into the positive part of the plane defined by the parabolic curve. As it can be observed from Fig. 1, all data are located into the overprediction region. This means that CHETAH software always overpredicts the value of the decomposition enthalpy: such a result is quite obvious because the software, as stated in Section 2.1, computes the set of products capable of maximizing the heat of decomposition. For what concern the scattering, only one functional group is located quite far from the parabolic line: epoxides. This means that, for such a particular functional group, CHETAH not only overestimates the real decomposition enthalpy value but also provides highly scattering predictions.

### 3.1. Nitro compounds

For what concerns this class, 54 nitro compounds have been analyzed (Table A1). Results have shown that for 7 of them there is disagreement between predicted (CHETAH) and experimental (DSC) energy release potentials. Particularly, for these compounds, CHETAH provided high ERP while DSC tests did not point out any instability. In these cases, CHETAH gave a conservative evaluation. As described before, DSC tests have been run up to 300 °C; this is the threshold temperature for the o-ring housed in the crucible. It is probable that some nitro compounds (reported with high ERP by CHETAH) can decompose at higher temperatures (not reached



**Fig. 1.** CHETAH performance for the prediction of the decomposition enthalpies of different functional groups, in terms of geometric mean (GM) and geometric variance (GV). The solid parabola is the minimum GV curve. Vertical continuous lines represent the “factor of two” agreement between predictions and experimental data.

during the DSC test). For the rest of the analyzed nitro compounds CHETAH correctly predicted a high or low ERP. For what concern the percentage error of theoretical predictions with respect to experimental results, it is possible to observe that CHETAH always tends to overestimate the decomposition enthalpy. This is in agreement with the methods used by CHETAH to calculate the heat of decomposition: it considers the set of decomposition products maximizing such a value. Finally, from Fig. 1, it is possible to observe, apart from the overestimation of the experimental value, a low scattering of the CHETAH predictions for this functional group.

### 3.2. Peroxides

All peroxides experimentally tested decomposed and CHETAH correctly predicted an HIGH energy released potential (Table A2). From Fig. 1 it is possible to observe that CHETAH predictions show the minimum scattering and overestimation: this means that the software is particularly able to provide conservative but reliable values of decomposition enthalpy for this particular class of compounds.

### 3.3. Epoxides

Among 9 examined epoxides, 8 of them decomposed and 1 resulted thermally stable (Table A3). CHETAH correctly predicted the associated risk. As stated before in Section 3, from Fig. 1 it is possible to observe, apart an overprediction, a high scattering of all decomposition enthalpies predicted by CHETAH. This means that, regardless the agreement in terms of ERP, the software do not provide reliable values of decomposition enthalpies for this particular class of compounds.

### 3.4. Aldehydes

A total of 17 aldehydes have been examined: 6 of them decomposed and 11 resulted thermally stable (Table A4). For 3 of them there is disagreement between CHETAH prediction and experimental DSC analysis. Anyway, CHETAH always gave a conservative evaluation in terms of ERP. From Fig. 1 it is possible to observe that CHETAH provides the worst predictions of decomposition enthalpy values but the scattering is minimum: this means that, regardless the overestimations, all predicted values can be considered reliable.

### 3.5. Nitriles

In total, 15 nitriles have been evaluated: 4 of them decomposed and 11 resulted thermally stable (Table A5). For 8 of them there is disagreement between CHETAH prediction and experimental DSC result. Anyway, CHETAH always gave a conservative evaluation in terms of ERP. From Fig. 1 a situation very similar to that one exhibits by the aldehydes functional group can be observed.

### 3.6. Acids

All the acids experimentally tested resulted thermally stable and CHETAH correctly predicted a LOW energy released potential (Table A6). For this functional group no statistical calculations have been performed because the percentage error was always equal to 100%.

### 3.7. Alcohols

Ten alcohols have been tested: 1 of them decomposed and 9 resulted thermally stable (Table A7). CHETAH correctly predicted the associated risk in terms of ERP. Even for this functional group no

statistical calculation has been performed because the percentage error was always equal to 100%.

### 3.8. Ketones

All the ketones experimentally tested resulted thermally stable and CHETAH correctly predicted a LOW energy released potential (Table A8). Even for this functional group no statistical calculation has been performed because the percentage error was always equal to 100%.

### 3.9. Hydrocarbon

All the hydrocarbons experimentally tested resulted thermally stable and CHETAH correctly predicted a LOW energy released potential (Table A9). Even for this functional group no statistical calculation has been performed because the percentage error was always equal to 100%.

### 3.10. Heterocyclic compounds

In total, 53 heterocyclic compounds have been examined: 12 of them decomposed and 41 resulted thermally stable (Table A10). For 13 of them there is disagreement between CHETAH prediction and experimental DSC analysis. Anyway, CHETAH always gave a conservative evaluation in terms of ERP. Observing Fig. 1 it is possible to state that there is always overestimation of the decomposition enthalpies but all predicted values are reliable.

### 3.11. Halogen compounds

A total of 45 halogen compounds have been evaluated: none of them decomposed (Table A11). For 1 of them there is disagreement between CHETAH and experimental DSC result. Once again CHETAH has given a conservative evaluation in terms of ERP. Even for this functional group no statistical calculation has been performed because the percentage error was always equal to 100%.

### 3.12. Ethers

All the ethers experimentally tested resulted thermally stable and CHETAH has been able to correctly predict a LOW energy released potential (Table A12). Even for this functional group no statistical calculation has been performed because the percentage error was always equal to 100%.

### 3.13. Esters

Fifteen esters have been examined: 1 of them decomposed and 14 resulted thermally stable (Table A13). Once again CHETAH has been able to correctly predict the associated risk. Even for this functional group no statistical calculation has been performed because the percentage error was always equal to 100%.

### 3.14. Amines

All the amines experimentally tested resulted thermally stable and CHETAH has been capable of correctly predicting a LOW energy released potential (Table A14). Even for this functional group no statistical calculation has been performed because the percentage error was always equal to 100%.

### 3.15. Amides

All the amides experimentally tested resulted thermally stable and CHETAH has been able to correctly predict a LOW energy released potential (Table A15). Even for this functional group no statistical calculation has been performed because the percentage error was always equal to 100%.

## 4. Conclusion

Aim of this work has been to compile a chemical risk database that can be as much complete as possible. Therefore 342 substances have been analyzed both theoretically, using CHETAH evaluation software, and experimentally, through the use of DSC and ARC equipments. Obtained results have been then compared in easy-to-consult tables (reported in the Annex).

With exception to nitriles and heterocyclic compounds classes, there is an almost full agreement (90.6%) between experimental (presence or not of thermal activity) and theoretically predicted ERP (high or low). Most of the disagreements (i.e. high ERP for CHETAH but lack of exothermic effects in the experimental tests) can be due to the employed experimental conditions (DSC maximum temperature is 300 °C). Probably, testing different kinds of crucibles and higher temperatures, the agreement would be wider. For what concern the prediction of the real decomposition enthalpies, CHETAH always provides overestimated values but for all analyzed functional groups except one (epoxides) the reliability is very high (minimum scattering).

As a conclusion, CHETAH software can be very useful as a first screening tool for thermochemical stability assessment of

compounds (in terms of ERP). It can be also used for a quick and easy compilation of a complete thermochemical risk assessment database with the only limitations that: 1) there will be always an overestimation of the predicted decomposition enthalpies and 2) for some functional groups, there could be a low reliability in the estimation because of a high scattering of the predicted values.

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The authors wish to express their gratitude and admiration to Dott. P. Cardillo, great scientist but, first of all, thermochemical pioneer, because of his fundamental contribution to the development of a complete physico-chemical background and a rigorous analytical method for all the most important aspects of thermochemical stability assessment. His pioneering work (Cardillo, 1988, 1994, 1998, 2001; Cardillo & Cattaneo, 1991; Cardillo, Gigante, Lunghi, Di Bari, & Ludovisi, 2002, 2008; Cardillo & Girelli, 1980, 1981, 1985a, 1985b, 1986), since the reconstruction and the detailed analysis of the Seveso accident (Cardillo & Girelli, 1980, 1981), has inspired many other works during the last twenty-five years (Di Somma et al., 2010; Dien et al., 1994; Fayet et al., 2011; Frurip et al., 1995; Lunghi et al., 2004; Sato & Sugawara, 1985; Sempere et al., 1997). Moreover, his deep interest in chemical process safety and hazards evaluation has been concretized in the technical organization of a great amount of conferences, conventions and workshops on these arguments. The authors hope that the fundamental contribution of this pioneer can continue to inspire newer and much more detailed studies on decompositions of chemical substances and their thermal stability in a great variety of storage, handling and process operating conditions.

## Annex. : Database

**Table A1**

Nitro compounds.

Compound	CAS	Formula	$\Delta H_f$ (kJ/mol)	$\Delta \hat{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta \hat{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
N-acetyl-3,5-dinitrotyrosine ethyl ester	29358-99-4	C <sub>13</sub> H <sub>15</sub> N <sub>3</sub> O <sub>8</sub>	-737.64	-3.43	HIGH	ARC	180	-1.67	51.3
Nifedipine	21829-25-4	C <sub>17</sub> H <sub>18</sub> N <sub>2</sub> O <sub>6</sub>	-705.3	-2.47	LOW	DSC	-	-	-
Nimodipine	66085-59-4	C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> O <sub>7</sub>	-942.45	-2.33	LOW	DSC	-	-	-
2-Nitro-1-propanol	2902-96-7	C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub>	-291.46	-4.31	HIGH	DSC	-	-	-
4-Bromobutyl nitrate	146563-40-8	C <sub>4</sub> H <sub>8</sub> BrNO <sub>3</sub>	-178.91	-2.12	HIGH	DSC	180	-1.07	49.5
3,4-Dichloronitrobenzene	99-54-7	C <sub>6</sub> H <sub>3</sub> Cl <sub>2</sub> NO <sub>2</sub>	8.79	-3.18	HIGH	ARC	-	-	-
1-Chloro-3,4-dinitrobenzene	610-40-2	C <sub>6</sub> H <sub>3</sub> ClN <sub>2</sub> O <sub>4</sub>	23.85	-4.64	HIGH	ARC	345	-1.8	61.2
2,4-difluoronitrobenzene	446-35-5	C <sub>6</sub> H <sub>3</sub> F <sub>2</sub> NO <sub>2</sub>	-310.87	-4.06	HIGH	ARC	330	-0.92	77.3
2,4-Dinitro-6-Bromoaniline	1817-73-8	C <sub>6</sub> H <sub>4</sub> BrN <sub>3</sub> O <sub>4</sub>	78.65	-3.68	HIGH	ARC	263	-0.63	82.9
2,4-Dichloro-6-nitroaniline	2683-43-4	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> NO <sub>2</sub>	15.06	-3.1	HIGH	ARC	320	-1.25	59.7
1,2,3-Trichloronitrobenzene	17700-09-3	C <sub>6</sub> H <sub>4</sub> Cl <sub>3</sub> NO <sub>2</sub>	-20.08	-2.59	HIGH	ARC	332	-0.67	74.1
4-Chloronitrobenzene	100-00-5	C <sub>6</sub> H <sub>4</sub> ClNO <sub>2</sub>	37.24	-3.76	HIGH	ARC	316	-1.76	53.2
4-Chloro-2-nitroaniline	89-63-4	C <sub>6</sub> H <sub>5</sub> ClN <sub>2</sub> O <sub>2</sub>	44.77	-3.56	HIGH	ARC	295	-2	43.8
2-Amino-4-chloro-5-nitrophenol	6358-07-2	C <sub>6</sub> H <sub>5</sub> ClN <sub>2</sub> O <sub>3</sub>	-133.89	-3.39	HIGH	ARC	160	-1	70.5
2-Amino-4-Nitrophenol	99-57-0	C <sub>6</sub> H <sub>5</sub> N <sub>2</sub> O <sub>4</sub>	-104.6	-4.02	HIGH	DSC	152	-0.84	79.1
Nitrobenzene	98-95-3	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	67.36	-4.64	HIGH	ARC	360	-1.76	62.1
2-Nitrophenol	88-75-5	C <sub>6</sub> H <sub>5</sub> NO <sub>3</sub>	-96.23	-4.35	HIGH	ARC	260	-2.13	51.0
2-Nitroaniline	88-74-4	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	63.6	-4.22	HIGH	ARC	280	-2	52.6
2,4-Dichloro-5-nitrobenzotrifluoride	400-70-4	C <sub>7</sub> H <sub>2</sub> Cl <sub>2</sub> F <sub>3</sub> N <sub>2</sub>	-674.00	-2.32	HIGH	DSC	-	-	-
4-Chloro-3,5-dinitrobenzotrifluoride	393-75-9	C <sub>7</sub> H <sub>2</sub> ClF <sub>3</sub> N <sub>2</sub> O <sub>4</sub>	-648.94	-3.58	HIGH	DSC	-	-	-
4-Chloro-3-nitrobenzotrifluoride	121-17-5	C <sub>7</sub> H <sub>3</sub> ClF <sub>3</sub> N <sub>2</sub> O <sub>2</sub>	-644.29	-2.73	HIGH	DSC	-	-	-
2-Chloro-3,5-dinitrobenzoic acids	2497-91-8	C <sub>7</sub> H <sub>3</sub> ClN <sub>2</sub> O <sub>6</sub>	-354.8	-3.89	HIGH	DSC	116	-4.14	-6.4
p-Nitrobenzoyl chloride	122-04-3	C <sub>7</sub> H <sub>4</sub> ClNO <sub>3</sub>	-119.24	-3.39	HIGH	DSC	277	-2.17	36.0
4-Chloro-3-nitrobenzoic acids	96-99-1	C <sub>7</sub> H <sub>4</sub> ClNO <sub>4</sub>	-340.99	-3.01	HIGH	ARC	327	-1.76	41.5
4-Nitrobenzotrifluoride	402-54-0	C <sub>7</sub> H <sub>4</sub> F <sub>3</sub> NO <sub>2</sub>	-604.17	-3.26	HIGH	ARC	-	-	-
4-Nitrobenzotrifluorides	619-72-7	C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	197.90	-4.6	HIGH	ARC	325	-1.71	62.8
2,4-Dinitrobenzoic acids	610-30-0	C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> O <sub>6</sub>	-325.93	-4.43	HIGH	ARC	298	-1.84	58.5
2-Nitrobenzoic acids	552-16-9	C <sub>7</sub> H <sub>5</sub> NO <sub>4</sub>	-304.18	-3.55	HIGH	ARC	230	-1.71	51.8
4-Fluoro-2-nitrotoluene	446-10-6	C <sub>7</sub> H <sub>6</sub> FNO <sub>2</sub>	-153.13	-4.02	HIGH	ARC	319	-0.84	79.1
4-Nitrobenzamide	619-80-7	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub>	-61.92	-3.97	HIGH	DSC	-	-	-
3,5-Dinitrobenzyl alcohol	71022-43-0	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>	-126.77	-5.03	HIGH	DSC	206	-3.47	31.0
2-Nitrotoluene	88-72-2	C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>	45.6	-4.27	HIGH	ARC	317	-1.71	60.0
p-Nitrotoluene	99-99-0	C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>	31	-4.16	HIGH	ARC	135	-2.829	32.0

Table A1 (continued)

Compound	CAS	Formula	$\Delta\bar{H}_f$ (kJ/mol)	$\Delta\bar{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\bar{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
6-Hydroxy-2-nitrotoluene	5460-31-1	C <sub>7</sub> H <sub>7</sub> NO <sub>3</sub>	-142.26	-3.93	HIGH	DSC	260	-0.85	78.4
3-Methyl-4-nitrophenol	2581-34-2	C <sub>7</sub> H <sub>7</sub> NO <sub>3</sub>	-143.09	-3.93	HIGH	ARC	181	-1	74.6
2-Nitroanisole	91-23-6	C <sub>7</sub> H <sub>7</sub> NO <sub>3</sub>	-84.51	-4.3	HIGH	ARC	328	-1.8	58.1
4-Nitro-3-cresol	2581-34-2	C <sub>7</sub> H <sub>7</sub> NO <sub>3</sub>	-151.04	-3.89	HIGH	DSC	234	-2.26	41.9
<i>p</i> -Nitro toluene sulfonic acids	121-03-9	C <sub>7</sub> H <sub>7</sub> NO <sub>5</sub> S	-527.06	-2.83	HIGH	ARC	145	-2.02	28.6
6-Methyl-2-nitroaniline	570-24-1	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>	41.42	-3.93	HIGH	DSC	280	-1	74.6
2-Methyl-3-nitroaniline	603-83-8	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>	38.61	-3.92	HIGH	DSC	-	-	-
2-Amino-4-nitroanisole	99-59-2	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O <sub>4</sub>	-84.93	-4.02	HIGH	DSC	260	-2.22	44.8
2,4-Dichloro-3,5-dinitrobenzotrifluoride	29091-09-6	C <sub>7</sub> HCl <sub>2</sub> F <sub>3</sub> N <sub>2</sub> O <sub>4</sub>	-689.48	-3.00	HIGH	DSC	378	-1.41	53.0
3,5-Dinitro-4-hydroxyphenylacetic acids	10463-37-3	C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> O <sub>7</sub>	-527.56	-4.07	HIGH	DSC	190	-0.148	96.4
3-Nitroacetophenone	121-89-1	C <sub>8</sub> H <sub>7</sub> NO <sub>3</sub>	-99.16	-3.89	HIGH	DSC	283	-1.84	52.7
4-Nitrobenzyl acetate	619-90-9	C <sub>9</sub> H <sub>9</sub> NO <sub>4</sub>	-326.77	-3.01	HIGH	DSC	170	-0.4	86.7
<i>p</i> -Nitrotoluic acids	104-03-0	C <sub>8</sub> H <sub>7</sub> NO <sub>4</sub>	-360.12	-3.23	HIGH	DSC	-	-	-
4-Hydroxy-3-nitroacetophenone	6322-56-1	C <sub>8</sub> H <sub>7</sub> NO <sub>4</sub>	-278.57	-3.68	HIGH	DSC	215	-0.76	79.3
5-Nitrovanillin	6635-20-7	C <sub>8</sub> H <sub>7</sub> NO <sub>5</sub>	-374.05	-3.89	HIGH	DSC	184	-2.3	40.9
3-Nitroacetanilide	122-28-1	C <sub>8</sub> H <sub>8</sub> NO <sub>3</sub>	-126.77	-3.51	HIGH	ARC	324	-2.05	41.6
6-Nitroquinoline	613-50-3	C <sub>9</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	-199.58	-4.14	HIGH	ARC	340	-1.42	65.7
8-Hydroxy-5-nitroquinoline	4008-48-4	C <sub>9</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub>	-41.00	-3.72	HIGH	DSC	247	-1.55	58.3
<i>o</i> -Nitrocinnamic acids	612-41-9	C <sub>9</sub> H <sub>7</sub> NO <sub>4</sub>	-250.2	-3.6	HIGH	DSC	256	-3.09	14.2
3-(4-Nitrophenyl)propionic acids	16642-79-8	C <sub>9</sub> H <sub>9</sub> NO <sub>4</sub>	-363.58	-3.18	HIGH	DSC	200	-1.4	56.0
Ethyl- <i>p</i> -nitrobenzoate	99-77-4	C <sub>9</sub> H <sub>9</sub> NO <sub>4</sub>	-340.49	-3.30	HIGH	DSC	-	-	-

Table A2

Peroxides.

Compound	CAS	Formula	$\Delta\bar{H}_f$ (kJ/mol)	$\Delta\bar{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\bar{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
Benzoyl peroxide	94-36-0	C <sub>14</sub> H <sub>10</sub> O <sub>4</sub>	-271.12	-3.01	HIGH	ARC	90	-1.84	38.9
Peroxyacetic acid	79-21-0	C <sub>2</sub> H <sub>4</sub> O <sub>3</sub>	-336.6	-4.52	HIGH	DSC	55	-2.04	54.8
<i>tert</i> -Butyl hydroperoxide	75-91-2	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	-246.01	-3.89	HIGH	DSC	85	-1.05	73.0
<i>tert</i> -Butylperoxide	110-05-4	C <sub>8</sub> H <sub>18</sub> O <sub>2</sub>	-348.94	-2.72	HIGH	ARC	102	-1.36	50.0
Cumene hydroperoxide	80-15-9	C <sub>9</sub> H <sub>12</sub> O <sub>2</sub>	-78.66	-3.64	HIGH	DSC	124	-1.88	48.4

Table A3

Epoxides.

Compound	CAS	Formula	$\Delta\bar{H}_f$ (kJ/mol)	$\Delta\bar{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\bar{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
4-(2,3-Epoxypropoxy)-carbazole	51997-51-4	C <sub>15</sub> H <sub>13</sub> NO <sub>2</sub>	-382.29	-3.209	HIGH	DSC	215	-8.5	-164.9
Ethylene Oxide	75-21-8	C <sub>2</sub> H <sub>4</sub> O	-52.72	-5.15	HIGH	ARC	320	-1.51	70.7
Epichlorohydrin	106-89-8	C <sub>3</sub> H <sub>5</sub> ClO	-107.94	-2.84	HIGH	ARC	375	-0.5	82.4
Propylene oxide	75-56-9	C <sub>3</sub> H <sub>6</sub> O	-92.47	-3.85	HIGH	ARC	340	-1.13	70.6
Epoxypropyl alcohol	556-52-5	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-239.74	-3.72	HIGH	ARC	62	-1.38	62.9
1,2-Epoxybutane	106-88-7	C <sub>4</sub> H <sub>8</sub> O	-110.04	-3.39	HIGH	ARC	145	-0.12	96.5
Cyclohexene oxide	286-20-4	C <sub>6</sub> H <sub>10</sub> O	-125.52	-2.72	LOW	DSC	-	-	-
Styrene oxide	96-09-3	C <sub>8</sub> H <sub>8</sub> O	39.75	-3.26	HIGH	ARC	252	-0.46	85.9
3-Fenoxy-1,2-epoxypropane	122-60-1	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	-112.97	-3.22	HIGH	ARC	320	-0.74	77.0

Table A4

Aldehydes.

Compound	CAS	Formula	$\Delta\bar{H}_f$ (kJ/mol)	$\Delta\bar{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\bar{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
Alpha-hexyl cinnamaldehyde	101-86-0	C <sub>15</sub> H <sub>20</sub> O	-113.8	-2.13	LOW	DSC	-	-	-
Acrolein	107-02-8	C <sub>3</sub> H <sub>4</sub> O	-80.75	-3.55	HIGH	ARC	70	-0.88	75.2
Methylglyoxal	78-98-8	C <sub>3</sub> H <sub>4</sub> O <sub>2</sub>	-270.29	-2.96	HIGH	DSC	40	-1.15	61.1
Propionaldehyde	123-38-6	C <sub>3</sub> H <sub>6</sub> O	-192.04	-2.13	LOW	DSC	-	-	-
Butanal	123-72-8	C <sub>4</sub> H <sub>8</sub> O	-208.41	-2.02	LOW	DSC	-	-	-
2-Ethylbutanal	97-96-1	C <sub>6</sub> H <sub>12</sub> O	-255.22	-1.71	LOW	DSC	-	-	-
2,2-Dimethyl-4-pentenal	5497-67-6	C <sub>7</sub> H <sub>12</sub> O	-158.99	-2.43	LOW	DSC	-	-	-
3,5-Dibromosalicylaldehyde	90-59-5	C <sub>7</sub> H <sub>4</sub> Br <sub>2</sub> O <sub>2</sub>	-168.19	-1.21	LOW	DSC	-	-	-
2-Chloro-6-fluorobenzaldehyde	387-45-1	C <sub>7</sub> H <sub>4</sub> ClFO	-257.32	-2.17	HIGH	ARC	302	-1.05	51.6
3-Fluorobenzaldehyde	456-48-4	C <sub>7</sub> H <sub>5</sub> FO	-280.33	-2.59	LOW	DSC	-	-	-
4-Fluorobenzaldehyde	459-57-4	C <sub>7</sub> H <sub>5</sub> FO	-234.64	-2.55	HIGH	DSC	-	-	-
<i>o</i> -Fluorobenzaldehyde	446-52-6	C <sub>7</sub> H <sub>5</sub> FO	-234.3	-2.55	HIGH	DSC	-	-	-
Benzaldehyde	100-52-7	C <sub>7</sub> H <sub>6</sub> O	-36.81	-2.63	HIGH	DSC	255	<sup>a</sup>	-
2,4-Dihydroxybenzaldehyde	95-01-2	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>	-389.11	-2.43	LOW	DSC	-	-	-
3-Phenylpropanal	104-53-0	C <sub>9</sub> H <sub>10</sub> O	-71.54	-2.38	LOW	DSC	-	-	-
3,4-Dimethoxybenzaldehyde	120-14-9	C <sub>9</sub> H <sub>10</sub> O <sub>3</sub>	-165.27	-2.84	HIGH	ARC	324	-0.42	85.2
Cinnamaldehyde	104-55-2	C <sub>9</sub> H <sub>8</sub> O	20.5	-2.84	HIGH	ARC	327	-0.5	82.4

<sup>a</sup> Decomposition enthalpy not entirely measured.

Table A5

Nitriles.

Compound	CAS	Formula	$\Delta\bar{H}_f$ (kJ/mol)	$\Delta\bar{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\bar{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
(3,4-Dimethoxyphenyl) acetonitrile	93-17-4	C <sub>10</sub> H <sub>11</sub> NO <sub>2</sub>	-126.36	-2.76	HIGH	ARC	346	-1.05	62.0
Chloro acetonitrile	107-14-2	C <sub>2</sub> H <sub>2</sub> ClN	87.86	-2.63	HIGH	DSC	–	–	–
Malononitrile	109-77-3	C <sub>3</sub> H <sub>2</sub> N <sub>2</sub>	249.8	-4.35	HIGH	ARC	180	-1.63	62.5
Fumaronitrile	764-42-1	C <sub>4</sub> H <sub>2</sub> N <sub>2</sub>	340.1	-4.85	HIGH	ARC	340	-0.46	90.5
Crotononitrile	4786-20-3	C <sub>4</sub> H <sub>5</sub> N	150.6	-3.64	HIGH	DSC	–	–	–
3-(Dimethylamino) propionitrile	1738-25-6	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub>	83.26	-2.76	LOW	DSC	–	–	–
Glutaronitrile	544-13-8	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub>	171.1	-3.01	HIGH	DSC	200	-0.92	69.4
3,5-Dichlorobenzonitrile	6575-00-4	C <sub>7</sub> H <sub>3</sub> Cl <sub>2</sub> N	159.4	-2.09	HIGH	DSC	–	–	–
2,6-Difluorobenzonitrile	1897-52-5	C <sub>7</sub> H <sub>3</sub> F <sub>2</sub> N	166.1	-5.23	HIGH	DSC	–	–	–
3,4-Dinitrobenzonitrile	4248-33-3	C <sub>7</sub> H <sub>3</sub> N <sub>3</sub> O <sub>4</sub>	184.1	-5.39	HIGH	ARC	360	-3.39	37.1
4-Fluorobenzonitrile	1194-02-1	C <sub>7</sub> H <sub>4</sub> FN	21.76	-2.88	HIGH	DSC	–	–	–
4-Trifluoromethylbenzonitrile	455-18-5	C <sub>8</sub> H <sub>4</sub> F <sub>3</sub> N	-463.13	-2.15	LOW	DSC	–	–	–
Isophthalonitrile	626-17-5	C <sub>8</sub> H <sub>4</sub> N <sub>2</sub>	364	-3.43	HIGH	DSC	–	–	–
1,4-Dicyanobenzene	623-26-7	C <sub>8</sub> H <sub>4</sub> N <sub>2</sub>	354.80	-1.37	HIGH	DSC	–	–	–
2-Chloro-6-methylbenzonitrile	6575-09-3	C <sub>8</sub> H <sub>6</sub> ClN	151.5	-2.21	LOW	DSC	–	–	–
Cinnamonitrile	4360-47-8	C <sub>9</sub> H <sub>7</sub> N	277.8	-3.18	HIGH	DSC	–	–	–

Table A6

Acids.

Compound	CAS	Formula	$\Delta\bar{H}_f$ (kJ/mol)	$\Delta\bar{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\bar{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
3-Benzoylpropionic acid	2051-95-8	C <sub>10</sub> H <sub>10</sub> O <sub>3</sub>	-478.23	-1.8	LOW	DSC	–	–	–
3-Hydroxy-4-methoxy cinnamic acid	537-73-5	C <sub>10</sub> H <sub>10</sub> O <sub>4</sub>	-567.35	-2.26	LOW	DSC	–	–	–
Lauric acid	143-07-7	C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>	-641.2	-1.075	LOW	DSC	–	–	–
5-(2,4-Difluorophenyl)salicylic acid	22494-42-4	C <sub>13</sub> H <sub>8</sub> F <sub>2</sub> O <sub>3</sub>	-784.92	-1.93	LOW	DSC	–	–	–
Flufenamic acid	530-78-9	C <sub>14</sub> H <sub>10</sub> F <sub>3</sub> NO <sub>2</sub>	-874.41	-1.70	LOW	DSC	–	–	–
Myristic acid	544-63-8	C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>	-682.87	-1.088	LOW	DSC	–	–	–
Palmitic acid	57-10-3	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	-723.8	-1.1	LOW	DSC	–	–	–
Oleic acid	112-80-1	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	-650.82	-1.392	LOW	DSC	–	–	–
Stearic acid	57-11-4	C <sub>18</sub> H <sub>36</sub> O <sub>2</sub>	-756.38	-1.109	LOW	DSC	–	–	–
Erucic acid	112-86-7	C <sub>22</sub> H <sub>42</sub> O <sub>2</sub>	-733.33	-1.36	LOW	DSC	–	–	–
Cholic acid	81-25-4	C <sub>24</sub> H <sub>40</sub> O <sub>5</sub>	-1314.70	-1.113	LOW	DSC	–	–	–
Glycolic acid	79-14-1	C <sub>2</sub> H <sub>4</sub> O <sub>3</sub>	-577.73	-1.36	LOW	DSC	–	–	–
1,3-Acetonedicarboxylic acid	542-05-2	C <sub>5</sub> H <sub>6</sub> O <sub>5</sub>	-974.45	-1	LOW	DSC	–	–	–
Adipic acid	124-04-9	C <sub>6</sub> H <sub>10</sub> O <sub>4</sub>	-864.83	-0.96	LOW	DSC	–	–	–
2-Ethylbutiric acid	88-09-5	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	-522.66	-0.95	LOW	DSC	–	–	–
Cyclohexanecarboxylic acid	98-89-5	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	-499.99	-1.29	LOW	DSC	–	–	–
2-Chlorobenzoic acid	118-91-2	C <sub>7</sub> H <sub>5</sub> ClO <sub>2</sub>	-319.23	-1.63	LOW	DSC	–	–	–
4-Hydroxybenzoic acid	99-96-7	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>	-487.85	-1.72	LOW	DSC	–	–	–
2-Hydroxybenzoic acid	69-72-7	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>	-487.85	-1.72	LOW	DSC	–	–	–
4-Hydroxybenzoic acid	99-96-7	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>	-487.85	-1.72	LOW	DSC	–	–	–
Cyclohexane-1,3-dicarboxylic acid	3971-31-1	C <sub>8</sub> H <sub>12</sub> O <sub>4</sub>	-876.12	-0.96	LOW	DSC	–	–	–
Isophthalic acid	121-91-5	C <sub>8</sub> H <sub>6</sub> O <sub>4</sub>	-696.21	-1.38	LOW	DSC	–	–	–
Terephthalic acid	100-21-0	C <sub>8</sub> H <sub>6</sub> O <sub>4</sub>	-706.26	-1.3	LOW	DSC	–	–	–
4-(Methylthio)benzoic acid	13205-48-6	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> S	-282.84	-1.63	LOW	DSC	–	–	–
2,4-Dimethoxybenzoic acid	91-52-1	C <sub>9</sub> H <sub>10</sub> O <sub>4</sub>	-611.7	-2.17	LOW	DSC	–	–	–
Isononanoic acid	26896-18-4	C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>	-608.77	-0.86	LOW	DSC	–	–	–
p-Fluorocinnamic acid	238-214-3	C <sub>9</sub> H <sub>7</sub> FO <sub>2</sub>	-431.96	-2.17	LOW	DSC	–	–	–
Cinnamic acid	621-82-9	C <sub>9</sub> H <sub>8</sub> O <sub>2</sub>	-225.93	-2.26	LOW	DSC	–	–	–
4-Hydroxyphenylpyruvic acid	156-39-8	C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>	-594.13	-2.09	LOW	DSC	–	–	–

Table A7

Alcohols.

Compound	CAS	Formula	$\Delta\bar{H}_f$ (kJ/mol)	$\Delta\bar{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\bar{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
2,4,6-Trimethylbenzyl alcohol	4170-90-5	C <sub>10</sub> H <sub>14</sub> O	-195.81	-1.8	LOW	DSC	–	–	–
2-Hydroxybiphenyl	90-43-7	C <sub>12</sub> H <sub>10</sub> O	3.43	-2.32	LOW	DSC	–	–	–
2,6-Diisopropylphenol	2078-54-8	C <sub>12</sub> H <sub>18</sub> O	-251.71	-1.62	LOW	DSC	–	–	–
Allyl alcohol	107-18-6	C <sub>3</sub> H <sub>6</sub> O	-131.8	-3.18	HIGH	ARC	360	-0.67	78.9
Isopropanol	67-63-0	C <sub>3</sub> H <sub>8</sub> O	-272.96	-1.35	LOW	DSC	–	–	–
Sorbitol	50-70-4	C <sub>6</sub> H <sub>14</sub> O <sub>6</sub>	-1139.2	-1.916	LOW	DSC	–	–	–
Phenol	108-95-2	C <sub>6</sub> H <sub>6</sub> O	-96.36	-2.37	LOW	DSC	–	–	–
Hydroquinone	123-31-9	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	-277.02	-2.22	LOW	DSC	–	–	–
Phloroglucinol	108-73-6	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub>	-445.6	-2.21	LOW	DSC	–	–	–
Guaiacol	90-05-1	C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>	-248.99	-2.49	LOW	DSC	–	–	–



**Table A8**

Ketones.

Compound	CAS	Formula	$\Delta\bar{H}_f$ (kJ/mol)	$\Delta\bar{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\bar{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
2',4'-Dimethoxyacetophenone	829-20-9	C <sub>10</sub> H <sub>12</sub> O <sub>3</sub>	-399.99	-2.43	LOW	DSC	–	–	–
4-tert-Butylcyclohexanone	98-53-3	C <sub>10</sub> H <sub>18</sub> O	-327.19	-1.38	LOW	DSC	–	–	–
3,4-Dimethoxyphenylacetone	776-99-8	C <sub>11</sub> H <sub>14</sub> O <sub>3</sub>	-417.14	-2.34	LOW	DSC	–	–	–
4-Bromobenzophenone	90-90-4	C <sub>13</sub> H <sub>9</sub> BrO	83.68	-1.8	LOW	DSC	–	–	–
2-Hydroxy-4-octyloxybenzophenone	1843-05-6	C <sub>21</sub> H <sub>26</sub> O <sub>3</sub>	-252.71	-2.05	LOW	DSC	–	–	–
Cyclopentanone	120-92-3	C <sub>5</sub> H <sub>8</sub> O	-194.14	-1.88	LOW	DSC	–	–	–
Mesityl oxide	141-79-7	C <sub>6</sub> H <sub>10</sub> O	-195.39	-2	LOW	DSC	–	–	–
Cyclohexanone	108-94-1	C <sub>6</sub> H <sub>10</sub> O	-230.12	-1.64	LOW	DSC	–	–	–
Acetylacetone	110-13-4	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>	-391.2	-1.8	LOW	DSC	–	–	–
3-Hexanone	589-38-8	C <sub>6</sub> H <sub>12</sub> O	-279.9	-1.5	LOW	DSC	–	–	–
2-Methyl-1,3-cyclopentanedione	765-69-5	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>	-337.65	-1.97	LOW	DSC	–	–	–
1,3-Cyclohexanedione	504-02-9	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>	-330.54	-2.05	LOW	DSC	–	–	–
2-Bromocyclohexanone	822-85-5	C <sub>6</sub> H <sub>9</sub> BrO	-220.91	-0.96	LOW	DSC	–	–	–
5-Methyl-5-propyl-[1,3]dioxan-2-one	7148-50-7	C <sub>8</sub> H <sub>14</sub> O <sub>3</sub>	-677.05	-1.25	LOW	DSC	–	–	–
2'-Chloroacetophenone	2142-68-9	C <sub>8</sub> H <sub>7</sub> ClO	-114.64	-1.92	LOW	DSC	–	–	–
Acetophenone	98-86-2	C <sub>8</sub> H <sub>8</sub> O	-87.03	-2.22	LOW	DSC	–	–	–
2'-Hydroxyacetophenone	118-93-4	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	-263.59	-2.17	LOW	DSC	–	–	–
4-Hydroxyacetophenone	99-93-4	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	-263.09	-2.17	LOW	DSC	–	–	–
2',4'-Dihydroxyacetophenone	89-84-9	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>	-439.32	-2.13	LOW	DSC	–	–	–
2-Hydroxypropiophenone	610-99-1	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	-285.34	-2.05	LOW	DSC	–	–	–
2-Methoxyacetophenone	579-74-8	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	-218.40	-2.51	LOW	DSC	–	–	–

**Table A9**

Hydrocarbons.

Compound	CAS	Formula	$\Delta\bar{H}_f$ (kJ/mol)	$\Delta\bar{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\bar{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
Butyl benzene	104-51-8	C <sub>10</sub> H <sub>14</sub>	-13.81	-1.84	LOW	DSC	–	–	–
Diphenylmethane	101-81-5	C <sub>13</sub> H <sub>12</sub>	138.1	-2.17	LOW	DSC	–	–	–
1-Phenylheptane	1078-71-3	C <sub>13</sub> H <sub>20</sub>	-75.73	-1.67	LOW	DSC	–	–	–
1-Tetradecene	1120-36-1	C <sub>14</sub> H <sub>28</sub>	-206.23	-1.612	LOW	DSC	–	–	–
1-Hexadecene	26952-14-7	C <sub>16</sub> H <sub>32</sub>	-249.59	-1.548	LOW	DSC	–	–	–
3,3-Dimethyl-1-butyne	917-92-0	C <sub>6</sub> H <sub>10</sub>	103.51	-3.53	HIGH	DSC	–	–	–
Ethyl Benzene	100-41-4	C <sub>8</sub> H <sub>10</sub>	29.71	-2.05	LOW	DSC	–	–	–
Isooctane	540-84-1	C <sub>8</sub> H <sub>18</sub>	-208.36	-1.13	LOW	DSC	–	–	–

**Table A10**

Heterocyclic compounds.

Compound	CAS	Formula	$\Delta\bar{H}_f$ (kJ/mol)	$\Delta\bar{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\bar{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
N-Phenylpiperazine	92-54-6	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub>	131	-2.43	LOW	DSC	–	–	–
Quinaldine	91-63-4	C <sub>10</sub> H <sub>9</sub> N	176.9	-2.43	LOW	DSC	–	–	–
3-Benzoylpyridine	5424-19-1	C <sub>12</sub> H <sub>9</sub> NO	163.2	-2.93	HIGH	DSC	–	–	–
Phenyl-4-pyridyl ketone	14548-46-0	C <sub>12</sub> H <sub>9</sub> NO	166.5	-2.93	HIGH	DSC	–	–	–
Dropropizine	17692-31-8	C <sub>13</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>	-240.41	-2.293	LOW	DSC	–	–	–
1,2,4-Triazole	288-88-0	C <sub>2</sub> H <sub>3</sub> N <sub>3</sub>	192.5	-3.59	HIGH	ARC	262	-1.09	69.6
Aziridine	151-56-4	C <sub>2</sub> H <sub>5</sub> N	126.3	-5.1	HIGH	ARC	100	-2.12	58.4
Isoxazole	288-14-2	C <sub>3</sub> H <sub>3</sub> NO	76.15	-4.89	HIGH	ARC	136	-1.34	72.6
Imidazole	288-32-4	C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>	146.4	-3.26	HIGH	DSC	–	–	–
Pyrazole	288-13-1	C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>	181.2	-3.76	HIGH	DSC	–	–	–
2,6-Dichloropyrazine	4774-14-5	C <sub>4</sub> H <sub>2</sub> Cl <sub>2</sub> N <sub>2</sub>	135.60	-2.13	HIGH	ARC	131	-1.17	45.1
Maleic anhydride	108-31-6	C <sub>4</sub> H <sub>2</sub> O <sub>3</sub>	-398.30	-2.42	HIGH	DSC	–	–	–
Pyrazine	290-37-9	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>	196.2	-3.39	HIGH	DSC	–	–	–
Pyridazine	289-80-5	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>	278.20	-4.39	HIGH	DSC	–	–	–
4,6-dihydroxy-2-mercaptopyrimidine	504-17-6	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> S	-130.12	-2.47	HIGH	DSC	–	–	–
2,4,5-Trihydroxypyrimidine	20636-41-3	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub>	-334.72	-2.72	HIGH	DSC	–	–	–
Thiophene	110-02-1	C <sub>4</sub> H <sub>4</sub> S	115.9	-2.26	LOW	DSC	–	–	–
2,4-Diamino-6-chloropyrimidine	156-83-2	C <sub>4</sub> H <sub>5</sub> ClN <sub>4</sub>	172	-2.34	HIGH	DSC	–	–	–
3-Methylisoxazole	30842-90-1	C <sub>4</sub> H <sub>5</sub> NO	33.89	-3.97	HIGH	ARC	171	-1.09	72.5
3-Amino-5-methylisoxazole	1072-67-9	C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O	20.92	-3.43	HIGH	ARC	140	-1.3	62.1
2,4-Diamino-6-iodoxypyrimidine	56-06-4	C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O	25.52	-2.72	HIGH	DSC	–	–	–
2,5-Dihydrofuran	1708-29-8	C <sub>4</sub> H <sub>6</sub> O	-66.94	-3.56	HIGH	DSC	–	–	–
Morpholine	110-91-8	C <sub>4</sub> H <sub>9</sub> NO	-142.72	-2.64	LOW	DSC	–	–	–
Tetrahydrofuran	142-68-7	C <sub>5</sub> H <sub>10</sub> O	-223.84	-1.97	LOW	DSC	–	–	–
Tetrahydrofurfuryl Alcohol	97-99-4	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	-369.02	-2.21	LOW	DSC	–	–	–
Piperidine	110-89-4	C <sub>5</sub> H <sub>11</sub> N	-48.95	-1.84	LOW	DSC	–	–	–
2-Chloro-5-nitropyridine	4548-45-2	C <sub>5</sub> H <sub>3</sub> ClN <sub>2</sub> O <sub>2</sub>	-8.37	-3.3	HIGH	ARC	344	-0.67	79.7
Pyridine	110-86-1	C <sub>5</sub> H <sub>5</sub> N	140.2	-2.97	HIGH	DSC	–	–	–
3-Hydroxypyridine	109-00-2	C <sub>5</sub> H <sub>5</sub> NO	-46.02	-2.63	HIGH	DSC	–	–	–

(continued on next page)

Table A10 (continued)

Compound	CAS	Formula	$\Delta\bar{H}_f$ (kJ/mol)	$\Delta\bar{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\bar{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
3-Aminopyridine	462-08-8	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub>	142.2	-2.72	HIGH	DSC	–	–	–
2-Amino-4-methylpyrimidine	108-52-1	C <sub>5</sub> H <sub>7</sub> N <sub>3</sub>	164	-2.72	HIGH	DSC	–	–	–
2-Hydrazinopyridine	4930-98-7	C <sub>5</sub> H <sub>7</sub> N <sub>3</sub>	263.2	-3.6	HIGH	ARC	165	-0.88	75.6
Furfurylamine	617-89-0	C <sub>5</sub> H <sub>7</sub> NO	-33.89	-3.1	HIGH	ARC	112	-0.92	70.3
4,5-Dimethyl isoxazole	7064-40-6	C <sub>5</sub> H <sub>7</sub> NO	-17.99	-3.58	HIGH	DSC	158	-8.30	131.8
N-Methylpyrrolidinone	872-50-4	C <sub>5</sub> H <sub>9</sub> NO	-195.39	-1.8	LOW	DSC	–	–	–
N-Aminoethylpiperazine	140-31-8	C <sub>6</sub> H <sub>15</sub> N <sub>3</sub>	20.92	-2.33	LOW	DSC	–	–	–
2-Cyanopyridine	100-70-9	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub>	274.9	-3.35	HIGH	DSC	–	–	–
3-Cyanopyridine	100-54-9	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub>	276.1	-3.39	HIGH	DSC	–	–	–
2-Chloro-6-methoxypyridine	17228-64-7	C <sub>6</sub> H <sub>6</sub> ClNO	-47.28	-2.38	HIGH	DSC	–	–	–
2-Methoxy-5-nitropyridine	5446-92-4	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub>	-128.44	-3.89	HIGH	ARC	314	-2.43	37.5
2-Methylpyridine	109-06-8	C <sub>6</sub> H <sub>7</sub> N	98.74	-2.47	LOW	DSC	–	–	–
4-(Hydroxymethyl)pyridine	586-95-8	C <sub>6</sub> H <sub>7</sub> NO	-50.63	-2.59	LOW	DSC	–	–	–
1-Methyl-2-pyridone	694-85-9	C <sub>6</sub> H <sub>7</sub> NO	-83.68	-2.3	LOW	DSC	–	–	–
1,2-(Methylenedioxy)benzene	274-09-9	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	-142.67	-3.1	HIGH	DSC	–	–	–
Sesamol	533-31-3	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>	-388.28	-2.44	LOW	DSC	–	–	–
4-Acetylpyridine	1122-54-9	C <sub>7</sub> H <sub>7</sub> NO	-31.38	-2.51	LOW	DSC	–	–	–
2,6-Dimethylpyridine	108-48-5	C <sub>7</sub> H <sub>9</sub> N	58.58	-2.13	LOW	DSC	–	–	–
1-(Cyanoacetyl)piperidine	15029-30-8	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O	-130.12	-1.97	LOW	DSC	–	–	–
Allyl piperidine	14446-67-4	C <sub>8</sub> H <sub>15</sub> N	6.69	-2.3	LOW	DSC	–	–	–
Desmetryne	1014-69-3	C <sub>8</sub> H <sub>15</sub> N <sub>5</sub> S	214.81	-2.318	LOW	DSC	–	–	–
Phthalic anhydride	85-44-9	C <sub>8</sub> H <sub>4</sub> O <sub>3</sub>	-371.54	-2.08	LOW	DSC	–	–	–
Quinoline	91-22-5	C <sub>9</sub> H <sub>7</sub> N	222.2	-2.72	HIGH	DSC	–	–	–
Tetrazole	288-94-8	CH <sub>2</sub> N <sub>4</sub>	334.3	-5.31	HIGH	ARC	145	-3.93	26.0

Table A11

Halogen compounds.

Compound	CAS	Formula	$\Delta\bar{H}_f$ (kJ/mol)	$\Delta\bar{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\bar{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
Neodecanoyl chloride	40292-82-8	C <sub>10</sub> H <sub>19</sub> ClO	-431.6	-1.05	LOW	DSC	–	–	–
4-(4-Fluorophenyl)-3-piperidinemethanol	216690-19-6	C <sub>12</sub> H <sub>16</sub> FNO	-320.83	-2.08	LOW	DSC	–	–	–
Lauroyl chloride	112-16-3	C <sub>12</sub> H <sub>23</sub> ClO	-452.5	-1.167	LOW	DSC	–	–	–
Bromodiphenylmethane	776-74-9	C <sub>13</sub> H <sub>11</sub> Br	169.9	-1.59	LOW	DSC	–	–	–
Bromohexine	3572-43-8	C <sub>14</sub> H <sub>20</sub> Br <sub>2</sub> N <sub>2</sub>	68.83	-1.27	LOW	DSC	–	–	–
3-Chloropropanenitriles	542-76-7	C <sub>3</sub> H <sub>4</sub> CIN	-28.87	-1.97	LOW	DSC	–	–	–
1-Bromo-3-chloropropane	109-70-6	C <sub>3</sub> H <sub>6</sub> BrCl	-108.36	-0.58	LOW	DSC	–	–	–
1-Bromo-4-chlorobutane	6940-78-9	C <sub>4</sub> H <sub>8</sub> BrCl	-128.87	-0.67	LOW	DSC	–	–	–
2-(2-Chloroethoxy)ethanol	628-89-7	C <sub>4</sub> H <sub>9</sub> ClO <sub>2</sub>	-422.16	-1.84	LOW	DSC	–	–	–
1-Chloro-2,3,4,5,6-pentabromo cyclohexane	25495-99-2	C <sub>6</sub> Br <sub>5</sub> Cl	-132.63	-0.29	LOW	DSC	–	–	–
2-Ethyl butanoyl chloride	2736-40-5	C <sub>6</sub> H <sub>11</sub> ClO	-334.72	-1.11	LOW	DSC	–	–	–
1,2-Dibromo-3,3-dimethylbutane	640-21-1	C <sub>6</sub> H <sub>12</sub> Br <sub>2</sub>	-161.25	-0.402	LOW	DSC	–	–	–
1,3-Dichlorobenzene	541-73-1	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	30.12	-1.71	LOW	DSC	–	–	–
2-Chloro benzofluoride	348-51-6	C <sub>6</sub> H <sub>4</sub> ClF	-143.93	-1.97	LOW	DSC	–	–	–
1,2-Difluorobenzene	367-11-3	C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>	-293.3	-2.51	HIGH	DSC	–	–	–
Fluoro benzene	462-06-6	C <sub>6</sub> H <sub>5</sub> F	-116.73	-2.38	LOW	DSC	–	–	–
2,4-Dichloro benzotrifluoride	320-60-5	C <sub>7</sub> H <sub>3</sub> Cl <sub>2</sub> F <sub>3</sub>	-658.52	-1.23	LOW	DSC	–	–	–
3,4-Dichloro benzotrifluoride	328-84-7	C <sub>7</sub> H <sub>3</sub> Cl <sub>2</sub> F <sub>3</sub>	-658.52	-1.23	LOW	DSC	–	–	–
2,4-Dichlorobenzotrifluoride	13014-18-1	C <sub>7</sub> H <sub>3</sub> Cl <sub>2</sub> F <sub>3</sub>	-69.04	-0.975	LOW	DSC	–	–	–
2-Chlorobenzoyl chloride	609-65-4	C <sub>7</sub> H <sub>4</sub> Cl <sub>2</sub> O	-39.33	-1.42	LOW	DSC	–	–	–
2-Chlorobenzotrifluoride	2136-89-2	C <sub>7</sub> H <sub>4</sub> Cl <sub>2</sub> F <sub>3</sub>	-39.32	-1.42	LOW	DSC	–	–	–
2-Chlorobenzotrifluoride	88-16-4	C <sub>7</sub> H <sub>4</sub> ClF <sub>3</sub>	-628.81	-1.531	LOW	DSC	–	–	–
4-Chlorobenzotrifluoride	98-56-6	C <sub>7</sub> H <sub>4</sub> ClF <sub>3</sub>	-628.81	-1.53	LOW	DSC	–	–	–
2-Fluorobenzoylchloride	393-52-2	C <sub>7</sub> H <sub>4</sub> ClFO	-331.37	-1.73	LOW	DSC	–	–	–
4-Fuorobenzoylchloride	403-43-0	C <sub>7</sub> H <sub>4</sub> ClFO	-331.37	-1.73	LOW	DSC	–	–	–
2,4-Dichlorobenzyl chloride	94-99-5	C <sub>7</sub> H <sub>5</sub> Cl <sub>3</sub>	-31.38	-1.46	LOW	DSC	–	–	–
Benzotrifluoride	98-08-8	C <sub>7</sub> H <sub>5</sub> F <sub>3</sub>	-599.11	-1.72	LOW	DSC	–	–	–
2-Chlorobenzyl chloride	611-19-8	C <sub>7</sub> H <sub>6</sub> Cl <sub>2</sub>	-8.37	-1.55	LOW	DSC	–	–	–
2-Chloro-6-fluorotoluene	443-83-4	C <sub>7</sub> H <sub>6</sub> ClF	-170.71	-2.3	LOW	DSC	–	–	–
4-Fluorobenzyl chloride	352-11-4	C <sub>7</sub> H <sub>6</sub> ClF	-174.05	-1.84	LOW	DSC	–	–	–
4-Fluorobenzamide	824-75-9	C <sub>7</sub> H <sub>6</sub> FNO	289.11	-2.01	LOW	DSC	–	–	–
2-Fluorobenzamide	445-28-3	C <sub>7</sub> H <sub>6</sub> FNO	289.11	-2.01	LOW	DSC	–	–	–
Benzyl chloride	100-44-7	C <sub>7</sub> H <sub>7</sub> Cl	18.83	-1.76	LOW	DSC	–	–	–
2-Fluorotoluene	95-52-3	C <sub>7</sub> H <sub>7</sub> F	-147.15	-2.14	LOW	DSC	–	–	–
4-Fluorotoluene	352-32-9	C <sub>7</sub> H <sub>7</sub> F	-147.15	-2.14	LOW	DSC	–	–	–
3-Fluorotoluene	352-70-5	C <sub>7</sub> H <sub>7</sub> F	-147.36	-2.14	LOW	DSC	–	–	–
1-Fluoro-4-methoxybenzene	459-60-9	C <sub>7</sub> H <sub>7</sub> FO	-270.2	-2.52	LOW	DSC	–	–	–
n-Octanoyl chloride	111-64-8	C <sub>8</sub> H <sub>15</sub> ClO	-369.99	-1.16	LOW	DSC	–	–	–
Hexachloro-m-xylene	881-99-2	C <sub>8</sub> H <sub>4</sub> Cl <sub>6</sub>	-135.14	-0.91	LOW	DSC	–	–	–
4-(Trifluoromethyl)benzoyl chloride	329-15-7	C <sub>8</sub> H <sub>4</sub> ClF <sub>3</sub> O	-816.26	-1.37	LOW	DSC	–	–	–
Xylene hexafluoride	402-31-3	C <sub>8</sub> H <sub>4</sub> F <sub>6</sub>	-1223.23	-1.531	LOW	DSC	–	–	–
p-Toluoyl chloride	874-60-2	C <sub>8</sub> H <sub>7</sub> ClO	-167.23	-1.56	LOW	DSC	–	–	–

Table A11 (continued)

Compound	CAS	Formula	$\Delta\bar{H}_f$ (kJ/mol)	$\Delta\bar{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\bar{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
2'-Fluoroacetophenone	445-27-2	C <sub>8</sub> H <sub>7</sub> FO	-280.32	-2.21	LOW	DSC	–	–	–
4-Acetotoluidide	103-89-9	C <sub>9</sub> H <sub>11</sub> NO	-144.35	-1.8	LOW	DSC	–	–	–
Isononanoyl chloride	36727-29-4	C <sub>9</sub> H <sub>17</sub> ClO	-419.86	-0.99	LOW	DSC	–	–	–

Table A12

Ethers.

Compound	CAS	Formula	$\Delta\bar{H}_f$ (kJ/mol)	$\Delta\bar{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\bar{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
1-Methoxycyclohexene	931-57-7	C <sub>7</sub> H <sub>12</sub> O	-272.79	-1.71	LOW	DSC	–	–	–
Veratrole	91-16-7	C <sub>8</sub> H <sub>10</sub> O <sub>2</sub>	-299.12	-2.65	LOW	DSC	–	–	–
Isopropoxyphenol	4812-20-8	C <sub>9</sub> H <sub>12</sub> O <sub>2</sub>	-321.58	-2.05	LOW	DSC	–	–	–
1,3,5-Trimethoxybenzene	621-23-8	C <sub>9</sub> H <sub>12</sub> O <sub>3</sub>	-384.93	-2.69	LOW	DSC	–	–	–

Table A13

Esters.

Compound	CAS	Formula	$\Delta\bar{H}_f$ (kJ/mol)	$\Delta\bar{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\bar{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
Methyl cinnamate	103-26-4	C <sub>10</sub> H <sub>10</sub> O <sub>2</sub>	-214.64	-2.34	LOW	DSC	–	–	–
Propyl benzoate	2315-68-6	C <sub>10</sub> H <sub>12</sub> O <sub>2</sub>	-333.46	-1.84	LOW	DSC	–	–	–
2-Ethylhexyl thioglycolate	7659-86-1	C <sub>10</sub> H <sub>20</sub> O <sub>2</sub> S	-533.88	-1.21	LOW	DSC	–	–	–
Dibutyl malonate	1190-39-2	C <sub>11</sub> H <sub>20</sub> O <sub>4</sub>	-919.7	1.25	LOW	DSC	–	–	–
Dibutyl fumarate	105-75-9	C <sub>12</sub> H <sub>20</sub> O <sub>4</sub>	-528.3	-1.623	LOW	DSC	–	–	–
Ethyl formate	109-94-4	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-371.12	-2	LOW	DSC	–	–	–
Methyl cyanoacetate	105-34-0	C <sub>4</sub> H <sub>5</sub> NO <sub>2</sub>	-236.81	-2.68	HIGH	ARC	289	-0.15	94.4
Allyl Acetate	591-87-7	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	-333.88	-2.26	LOW	DSC	–	–	–
Methyl acetoacetate	105-45-3	C <sub>5</sub> H <sub>8</sub> O <sub>3</sub>	-691.61	-1.51	LOW	DSC	–	–	–
Ethyl 2-chloroacetoacetate	609-15-4	C <sub>6</sub> H <sub>9</sub> ClO <sub>3</sub>	-635.97	-1.3	LOW	DSC	–	–	–
3-Hydroxyquinuclidine	1619-34-7	C <sub>7</sub> H <sub>13</sub> NO	-218.57	1.799	LOW	DSC	–	–	–
Ethyl benzoate	93-89-0	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	-284.09	-2.09	LOW	DSC	–	–	–
Phenyl propionate	211-282-1	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	-299.57	-1.97	LOW	DSC	–	–	–
Aceclidine	212-574-1	C <sub>9</sub> H <sub>15</sub> NO <sub>2</sub>	-267.94	-2.489	LOW	DSC	–	–	–
1,5-Diethyl-2-aminopentanedioate	10310-46-0	C <sub>9</sub> H <sub>17</sub> NO <sub>4</sub>	-829.69	-1.50	LOW	DSC	–	–	–

Table A14

Amines.

Compound	CAS	Formula	$\Delta\bar{H}_f$ (kJ/mol)	$\Delta\bar{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\bar{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
1,2-Diphenylethylamine	25611-78-3	C <sub>14</sub> H <sub>15</sub> N	162.3	-2.26	LOW	DSC	–	-0	–
2,2'-Diaminobenzyl	34124-14-6	C <sub>14</sub> H <sub>16</sub> N <sub>2</sub>	187.9	-2.26	LOW	DSC	–	–	–
N,N-dibutylaniline	613-29-6	C <sub>14</sub> H <sub>23</sub> N	-46.02	-1.88	LOW	DSC	–	–	–
N,N-dimethylaurylamine	112-18-5	C <sub>14</sub> H <sub>31</sub> N	-258.32	-1.504	LOW	DSC	–	–	–
Stearylamine	124-30-1	C <sub>18</sub> H <sub>39</sub> N	-379.74	-1.293	LOW	DSC	–	–	–
2-Diethylaminoethyl diphenyl acetate	64-95-9	C <sub>20</sub> H <sub>25</sub> NO <sub>2</sub>	-250.61	-2	LOW	DSC	–	–	–
Tribenzylamine	620-40-6	C <sub>21</sub> H <sub>21</sub> N	305.4	-2.43	LOW	DSC	–	–	–
Ethylenediamine	107-15-3	C <sub>2</sub> H <sub>8</sub> N <sub>2</sub>	-15.06	-2.23	LOW	DSC	–	–	–
Allylamine	107-11-9	C <sub>3</sub> H <sub>7</sub> N	28.87	-2.8	LOW	DSC	–	–	–
Propyl amine	107-10-8	C <sub>3</sub> H <sub>9</sub> N	-72.38	-1.63	LOW	DSC	–	–	–
2-Methoxyethylamine	109-85-3	C <sub>3</sub> H <sub>9</sub> NO	-184.10	-2.51	LOW	DSC	–	–	–
n-Butylamine	109-73-9	C <sub>4</sub> H <sub>11</sub> N	-92.05	-1.34	LOW	DSC	–	–	–
2-Aminomethyl propanol	124-68-5	C <sub>4</sub> H <sub>11</sub> NO	-271.12	-1.54	LOW	DSC	–	–	–
2-Dimethylaminoethanol	108-01-0	C <sub>4</sub> H <sub>11</sub> NO	-203.34	-2.3	LOW	DSC	–	–	–
2-Amino-2-methyl-1-propanol	124-68-5	C <sub>4</sub> H <sub>11</sub> NO	-271.12	-1.55	LOW	DSC	–	–	–
2-(2-Aminoethoxy)ethanol	929-06-6	C <sub>4</sub> H <sub>11</sub> NO <sub>2</sub>	-364.43	-2.38	LOW	DSC	–	–	–
Cyclohexyl amine	108-91-8	C <sub>6</sub> H <sub>13</sub> N	-105.01	-1.38	LOW	DSC	–	–	–
N-aminohexamethyleneimine	5906-35-4	C <sub>6</sub> H <sub>14</sub> N <sub>2</sub>	-79.91	-1.59	LOW	DSC	–	–	–
2,4,6-Tribromobenzeneamine	147-82-0	C <sub>6</sub> H <sub>4</sub> Br <sub>3</sub> N	154.8	-0.84	LOW	DSC	–	–	–
2,4-Dibromoaniline	615-57-6	C <sub>6</sub> H <sub>5</sub> Br <sub>2</sub> N	132.20	-1.04	LOW	DSC	–	–	–
o-Bromoaniline	615-36-1	C <sub>6</sub> H <sub>6</sub> BrN	109.60	-1.46	LOW	DSC	–	–	–
3-Chloroaniline	108-42-9	C <sub>6</sub> H <sub>6</sub> ClN	57.32	-1.92	LOW	DSC	–	–	–
2-Amino-4-chlorophenol	95-85-2	C <sub>6</sub> H <sub>6</sub> ClNO	-118.82	-1.88	LOW	DSC	–	–	–
Aniline	62-53-3	C <sub>6</sub> H <sub>7</sub> N	87.02	-1.8	LOW	DSC	–	–	–
4-Aminophenol	123-30-8	C <sub>6</sub> H <sub>7</sub> NO	-89.11	-2.26	LOW	DSC	–	–	–
3,4-Diaminotoluene	496-72-0	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub>	57.73	-2	LOW	DSC	–	–	–
Diethylaminoacetone	1620-14-0	C <sub>7</sub> H <sub>15</sub> NO	-222.59	-2.05	LOW	DSC	–	–	–
2,6-Dichloro-3-methylaniline	64063-37-2	C <sub>7</sub> H <sub>7</sub> Cl <sub>2</sub> N	-2.93	-1.55	LOW	DSC	–	–	–
Benzylamine	100-46-9	C <sub>7</sub> H <sub>9</sub> N	62.34	-2.13	LOW	DSC	–	–	–
N-Methylaniline	100-61-8	C <sub>7</sub> H <sub>9</sub> N	85.35	-2.38	LOW	DSC	–	–	–

(continued on next page)

Table A14 (continued)

Compound	CAS	Formula	$\Delta\hat{H}_f$ (kJ/mol)	$\Delta\hat{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\hat{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
2-Methoxyaniline	90-04-0	C <sub>7</sub> H <sub>9</sub> NO	58.58	-2.55	LOW	DSC	–	–	–
N,N-Dimethylaniline	121-69-7	C <sub>8</sub> H <sub>11</sub> N	84.1	-2.38	LOW	DSC	–	–	–
3-Methoxybenzylamine	5071-96-5	C <sub>8</sub> H <sub>11</sub> NO	-71.55	-2.47	LOW	DSC	–	–	–
2,4-Dimethoxyaniline	2735-04-8	C <sub>8</sub> H <sub>11</sub> NO <sub>2</sub>	-225.52	-2.55	LOW	DSC	–	–	–
Benzocaine	94-09-7	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>	-237.57	-1.78	LOW	DSC	–	–	–
N,N-dimethyl-p-toluidine	99-97-8	C <sub>9</sub> H <sub>13</sub> N	66.94	-2.3	LOW	DSC	–	–	–
N-ethyl-N-methylaniline	613-97-8	C <sub>9</sub> H <sub>13</sub> N	12.55	-2.26	LOW	DSC	–	–	–
N-ethyl-o-toluidine	94-68-8	C <sub>9</sub> H <sub>13</sub> N	25.94	-2	LOW	DSC	–	–	–
Trimethylaniline	88-05-1	C <sub>9</sub> H <sub>13</sub> N	-4.18	-1.76	LOW	DSC	–	–	–
2-(2-Methoxyphenoxy)ethylamine	1836-62-0	C <sub>9</sub> H <sub>13</sub> NO <sub>2</sub>	-228.36	-2.53	LOW	DSC	–	–	–

Table A15

Amides.

Compound	CAS	Formula	$\Delta\hat{H}_f$ (kJ/mol)	$\Delta\hat{H}_{dec, max}$ (kJ/g)	ERP	Instrument	$T_{on}$ (°C)	$\Delta\hat{H}_{dec}$ (kJ/g)	$\epsilon$ (%)
Acetoacetanilide	102-01-2	C <sub>10</sub> H <sub>11</sub> NO <sub>2</sub>	-274.05	-1.92	LOW	DSC	–	–	–
4-Acetophenetidine	62-44-2	C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub>	-301.25	-1.97	LOW	DSC	–	–	–
2-Acetoacetotoluidide	93-68-5	C <sub>11</sub> H <sub>13</sub> NO <sub>2</sub>	-307.52	-1.8	LOW	DSC	–	–	–
2-Acetoacetanisidide	92-15-9	C <sub>11</sub> H <sub>13</sub> NO <sub>3</sub>	-430.53	-2.05	LOW	DSC	–	–	–
Atenolol	29122-68-7	C <sub>14</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>	-535.68	-1.832	LOW	DSC	–	–	–
p-Chlorobenzoyl tyramine	41859-57-8	C <sub>15</sub> H <sub>14</sub> ClNO <sub>2</sub>	-209.83	-1.937	LOW	DSC	–	–	–
Acetamide	60-35-5	C <sub>2</sub> H <sub>5</sub> NO	-238.07	-1	LOW	DSC	–	–	–
Ethylene bis(stearamide)	110-30-5	C <sub>38</sub> H <sub>76</sub> N <sub>2</sub> O <sub>2</sub>	-1117.38	-1.197	LOW	DSC	–	–	–
N,N-Dimethyl formamide	68-12-2	C <sub>3</sub> H <sub>7</sub> NO	-191.62	-1.8	LOW	DSC	–	–	–
Propionamide	79-05-0	C <sub>3</sub> H <sub>7</sub> NO	-264.01	-0.96	LOW	DSC	–	–	–
Diacetamide	625-77-4	C <sub>4</sub> H <sub>7</sub> NO <sub>2</sub>	-436.81	-1	LOW	DSC	–	–	–
Succinamide	110-14-5	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>	-442.25	-0.98	LOW	DSC	–	–	–
N,N-dimethylacetamide	127-19-5	C <sub>4</sub> H <sub>9</sub> NO	-225.1	-1.71	LOW	DSC	–	–	–
p-Trifluoromethylbenzamide	6575-09-3	C <sub>8</sub> H <sub>6</sub> F <sub>3</sub> NO	-774.00	-1.59	LOW	DSC	–	–	–
Acetanilide	103-84-4	C <sub>8</sub> H <sub>9</sub> NO	-128.44	-1.8	LOW	DSC	–	–	–

## References

- ASTM E (1981). Standard guide for assessing the thermal stability of materials by methods of accelerating rate calorimetry.
- ASTM E 537. Standard test method for assessing the thermal stability of chemicals by methods of thermal analysis.
- Barontini, F., Cozzani, V., & Petarca, L. (2001). Thermal stability and decomposition products of hexabromocyclododecane. *Industrial & Engineering Chemistry Research*, 40(15), 3270–3280.
- Benson, S. W. (1976). *Thermochemical kinetics*. New York: Wiley & Sons.
- Bretherick, L. (1999). *Handbook of reactive chemical hazards*. London: Butterworth-Heinemann.
- Cardillo, P. (1988). Thermal-decomposition of isoxazoles. *Chimica & L Industria*, 70(6), 90–92.
- Cardillo, P. (1994). Calorimetric data for hazard process assessment – alkene epoxidation with peracids. *Journal of Loss Prevention in the Process Industries*, 7(1), 33–37.
- Cardillo, P. (1998). *Incidenti in ambiente chimico- Guida allo studio e alla valutazione delle reazioni fuggitive*. San Donato Milanese: Stazione sperimentale per i Combustibili.
- Cardillo, P. (2001). Some historical accidental explosions. *Journal of Loss Prevention in the Process Industries*, 14(1), 69–76.
- Cardillo, P., & Cattaneo, M. (1991). Application of DSC with atmospheric control in thermal hazard evaluation: a discussion of the sources of error. *Journal of Loss Prevention in the Process Industries*, 4, 283–286.
- Cardillo, P., Gigante, L., Lunghi, A., Di Bari, C., & Ludovisi, G. (2002). Thermodynamic for chemical safety: predictive criteria of thermal instability. *Rivista dei Combustibili*, 56, 4–5.
- Cardillo, P., Gigante, L., Lunghi, A., Fraloni Morgera, A., & Zanirato, P. (2008). Hazardous N-containing system: thermochemical and computational evaluation of the intrinsic molecular reactivity of some aryl azides and diazides. *New Journal of Chemistry*, 32(1), 47–53.
- Cardillo, P., Gigante, L., Lunghi, A., & Zanirato, P. (2010). Revisiting the thermal decomposition of five ortho-substituted phenyl azides by calorimetric techniques. *Journal of Thermal Analysis and Calorimetry*, 100(1), 191–198.
- Cardillo, P., & Girelli, A. (1980). Studio termooanalitico della miscela di Seveso. *Chimica & L Industria*, 62, 651.
- Cardillo, P., & Girelli, A. (1981). The Seveso runaway reaction – a thermoanalytical study. *Institution of Chemical Engineers Symposium Series*, 68, 3N1.
- Cardillo, P., & Girelli, A. (1985a). Thermal-stability of dimethylacetamide-carbon tetrachloride mixtures. *Thermochemical Acta*, 82, 339–342.
- Cardillo, P., & Girelli, A. (1985b). Thermal-stability of chloronitrobenzyl halogenides. *Chimica & L Industria*, 67(7–8), 403–405.
- Cardillo, P., & Girelli, A. (1986). Thermal-stability of nitrobenzyl alcohols. *Chimica & L Industria*, 68(6), 68–70.
- Copelli, S., Derudi, M., Lunghi, A., Pasturezzi, C., & Rota, R. (2011b). Experimental design of topological curves to safely optimize highly exothermic complex reacting systems. *Industrial & Engineering Chemistry Research*, 50, 9910–9917.
- Copelli, S., Derudi, M., Sempere, J., Serra, E., Lunghi, A., Pasturezzi, C., et al. (2011a). Emulsion polymerization of vinyl acetate: safe optimization of a hazardous complex process. *Journal of Hazardous Materials*, 192, 8–17.
- Di Somma, L., Pollio, A., Pinto, G., De Falco, M., Pizzo, E., & Andreozzi, R. (2010). A procedure for the assessment of the toxicity of intermediates and products formed during the accidental thermal decomposition of a chemical species. *Journal of Hazardous Materials*, 176(1–3), 575–578.
- Dien, J. M., Fierz, H., Stoessel, F., & Kille, G. (1994). The thermal risk of autocatalytic decompositions – a kinetic-study. *Chimia*, 48(12), 542–550.
- Fayet, G., Rotureau, P., Joubert, L., & Adamo, C. (2011). Development of a QSPR model for predicting thermal stabilities of nitroaromatic compounds taking into account their decomposition mechanisms. *Journal of Molecular Modelling*, 17(10), 2443–2453.
- Fox, D. G. (1984). Uncertainty in air quality modeling. *Bulletin of the American Meteorological Society*, 65, 27–36.
- Frupip, D. J., Chakrabarti, A., Dowe, J. R., Ferguson H. D., Gupta, S. K., Hofelich, T. C., et al. (1995). Determination of chemical process heats by experiment and prediction. (Boston: International Symposium of Runaway Reactions and Pressure Relief Design).
- Hanna, S. R. (1993). Uncertainties in air quality model predictions. *Boundary-layer Meteorology*, 62(1–4), 3–20.
- Harrison, B. K., Madas, A., & Sharma, A. (2005). *CHETAH 8.0 users manual, the ASTM computer program for chemical thermodynamics and energy release evaluation*. West Conshohocken: ASTM.

- Lunghi, A., Gigante, L., Cardillo, P., Stefanoni, V., Pulga, G., & Rota, R. (2004). Hazard assessment of substances produced from the accidental heating of chemical compounds. *Journal of Hazardous Materials*, 116(1–2), 11–21.
- Maestri, F., Copelli, S., Rota, R., Gigante, L., Lunghi, A., & Cardillo, P. (2009). Simple procedure for optimal scale-up of fine chemical processes. II. Nitration of 4-chlorobenzotrifluoride. *Industrial & Engineering Chemistry Research*, 48(3), 1316–1324.
- Roduit, B., Borgeat, Ch., Berger, B., Folly, P., Alonso, B., & Aebischer, J. N. (2005). The prediction of thermal stability of self-reactive chemicals. *Journal of Thermal Analysis and Calorimetry*, 80, 91–102.
- Sato, H., & Sugawara, S. (1985). Thermal-stability and decomposition mechanism of diazonium tetraphenylborate (diazo tpb salt). *Thermochemica Acta*, 93, 113–116.
- Seaton, W. H., Freedman, E., & Treweek, D. N. (1974). *CHETAH – The ASTM chemical thermodynamic and energy release potential evaluation program*. Philadelphia: ASTM.
- Sempere, J., Nomen, R., Serra, R., & Cardillo, P. (1997). Thermal hazard assessment using closed-cell adiabatic calorimetry. *Journal of Loss Prevention in the Process Industries*, 10(1), 55–62.
- Stoessel, F. (2008). *Thermal safety of chemical processes*. Weinheim: Wiley-WCH.
- Treweek, D. N., Pardue, W. M., Hoyland, J. R., Alexander, C. A., Seaton, W. H., & Freedman, E. (1978). Estimation of explosive hazard by computer. *Ohio Journal of Science*, 78, 245–254.