

DIADEM Professional

File Edit View Format Tools Windows About Help

DIPPR Database: C:\Program Files\DIPPR801\Databases\DIPPR801_Jan2010.mdb

DIPPR Information and Data Evaluation Manager

User Database:

Name: DIPPR ID: CASN: Formula: Retrieve Clear

T. Dep. Graph Cons Constants T Dep. Grid T Dep Props Data: Const Data: T Dep.

Filter Sort Switch all T. Dep. properties to: Density, Liquid

Window Control

- Search
 - BENZENE (501)
 - Information
 - Predictions
 - CAFFEINE (6853)
 - Information
 - Constants
 - T. Dep. Grid
 - T. Dep. Proper
 - Data: Constant
 - Data: T-dep.
 - References
 - Structure
 - Predictions
 - PHENOL (1181)
 - Information
 - Predictions
 - Data Tools
 - Add/Edit Data
 - Temperature Charts
 - Comparisons
 - Options

Search

Search Mode

- Name
 - DIPPR-ID
 - Formula
 - CAS Number
 - Property
- Carbon # Constraint
 - Any

Family Names

- All Families
- Acetates
- Acids, Aromatic Carboxylic
- Acids, Dicarboxylic
- Acids, Inorganic
- Acids, n-Aliphatic
- Acids, Other Aliphatic
- Acids, Polyfunctional
- Alcohols, Aromatic
- Alcohols, Cycloaliphatic
- Alcohols, n-
- Alcohols, Other Aliphatic
- Aldehydes
- Alkanes, n-

General Searches

Name: PHENOL

- "Exact" Match
- "Partial" Match

Search within results

Search

Results: PHENOL Total Compounds Found: 1

Submit Search Select All Deselect All

DIPPR - PHENOL - T Dependent Properties

Property: Density, Liquid Temperature Range: 314.06 to 694.25 K

EQUATION 105

$$Y = \frac{A}{B \left(1 + \frac{T - T_0}{T_0} \right)^n}$$

Coefficients

Units	kmol/m ³
A	1.3798
B	0.31598
C	694.25
D	0.32768
E	0
Error	< 1%

Note:

Calculator

Temperature: Value: Calculate

Value: kmol/m³

Temperature Range

From 314.06 to 694.25 with 20

T/K	kmol/m ³
314.06	11.2435
334.07	11.0583
354.08	10.86328
374.09	10.67606
394.10	10.47819
414.11	10.27517
434.12	10.06637
454.13	9.85106

Points Increment Reset Values

Tabulate Graph

DIPPR - PHENOL - Constants

DIPPR Name: PHENOL CASN: 108-95-2 Formula: C₆H₆O

Family Name: AROMATIC ALCOHOLS

IUPAC Name: PHENOL

Chem Abstract Name: PHENOL

Structure (C₆H₅)OH

SMILES Formula: c1ccccc1O

DIPPR ID: 1181

Synonyms: BENZENE, HYDROXY-; BENZENOL; BENZOPHENOL; CARBOLIC ACID; HYDROXYBENZENE; MONOHYDROXYBENZENE; PHENYL ALCOHOL

Accepted

Property	Value	Units	Ref	Notes	Data Type	Uncertainty
Molecular Weight	94.11124	kg/kmol	1	2441		
Critical Temperature	694.25	K	406		Experimental	< 1%
Critical Pressure	6.130E+06	Pa	406		Experimental	< 3%
Critical Volume	0.229	m ³ /kmol	406		Experimental	< 5%
Critical Compressibility Factor	0.243		406		Defined	
Melting Point	314.06	K	0	725	Predicted	< 1%
Triple Point Temperature	314.06	K	21		Experimental	< 1%

Density, Liquid

Print Copy Sort Format Axis Format Data Format Graph View

PHENOL

Correlation 9220

Raw Data

A: Kudchadker, A.P.

A: Timmermans, J.

A: Anonymous

A: Anonymous

N: Smith, B.D.

Constants

Predictions

Density, Liquid

T	Value
323.15	11.155
333.15	11.065
353.15	10.884
373.15	10.695
393.15	10.498

Reference: [406] Kudchadker, A.P., Kudchadker, S.A., Wilhoit, R.C., "Key Chemicals Data Book-5, Phenol," Thermodynamics

Uncertainty: < 1% (Staff)

Type: Smoothed (Evaluated)

Pen: [20] Color: [Blue]

Style: x Size: 100

DIADEM is the official interface for the DIPPR® 801 database. Using DIADEM, users can view 2D and 3D images of compounds, plot constant and temperature dependent data and correlations, predict values for compounds using a variety of prediction methods, plus thousands of other options.

Search

Search Mode

- ☐ Name
- ☐ DIPPR-ID
- ☐ Formula
- ☐ CAS Number*
- ☒ Property

Family Names:

- ☒ All Families
- ☐ Acetates
- ☐ Acids, Aromatic Carboxylic
- ☐ Acids, Dicarboxylic
- ☐ Acids, Inorganic
- ☐ Acids, n-Aliphatic
- ☐ Acids, Other Aliphatic
- ☐ Acids, Polyfunctional
- ☐ Alcohols, Aromatic
- ☐ Alcohols, Cycloaliphatic

General Searches

Partial Name:

☐ "Exact" Match
☐ "Partial" Match

☐ Search within results

Carbon # Constraint

> or =

Constant Searches

Property	Min	Max	Units	Type	Error
Molecular Weight	52	72	kg/kmol	Any	ALL

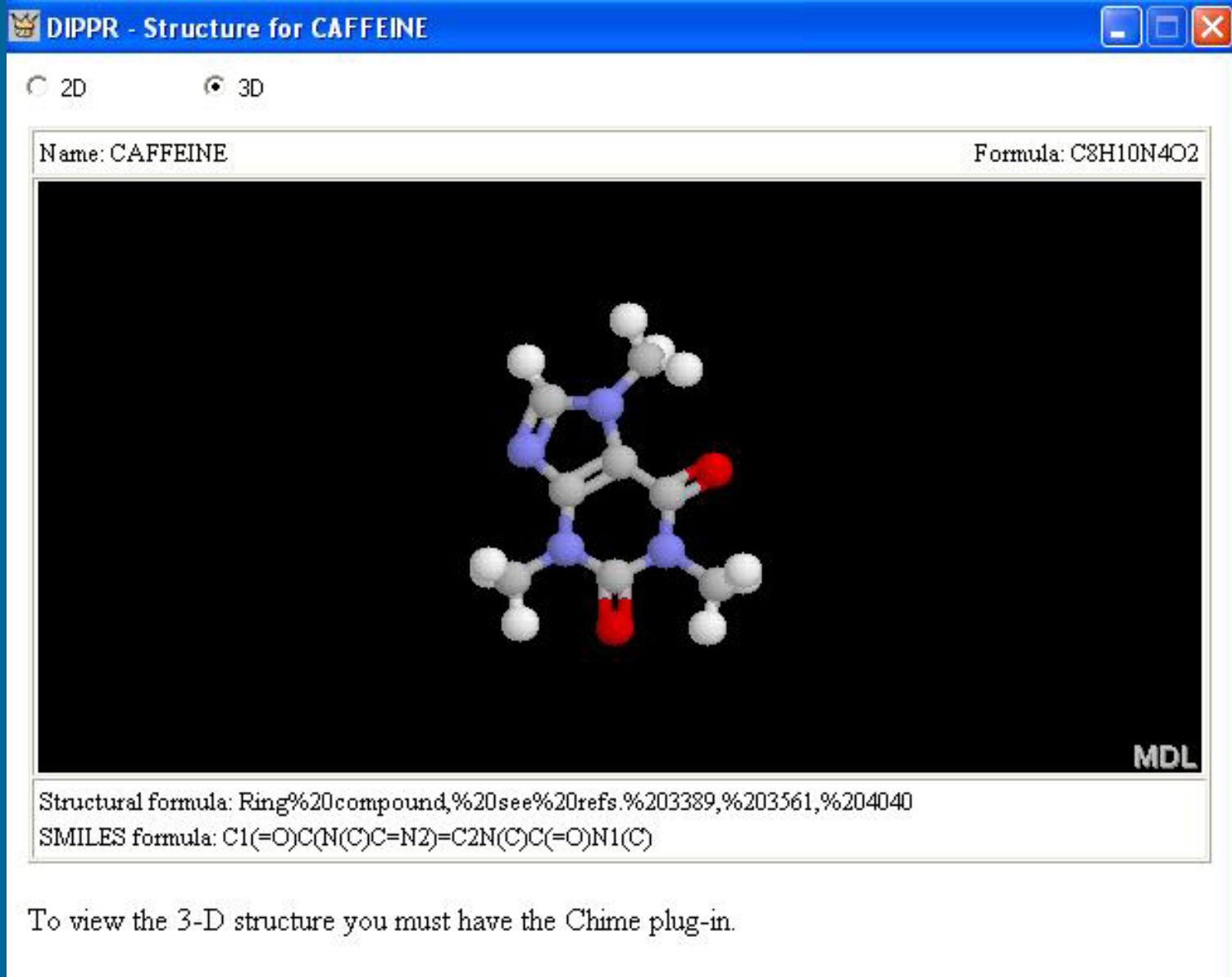
Search

Results: Total Compounds Found: 105





☐ METHANE
☒ DIPHENYLMETHANE
☐ TRIPHENYLMETHANE
☐ TETRAPHENYLMETHANE
☐ DICHLOROMETHANE
☐ CHLOROFLUOROMETHANE
☐ DICHLORODIFLUOROMETHANE
☐ TRICHLOROFLUOROMETHANE

*CAS Registry Number® is a Registered Trademark of the American Chemical Society

DIADEM's search capabilities include searching by compound name, formula, CAS #, carbon constraints, as well as by user-defined property criteria as is shown here.



Users can view compound structures in 2- or 3-D and can rotate the compound in 3-D for viewing at many different angles.


DIPPR - DIPHENYLMETHANE - T Dependent Properties




Property
Vapor Pressure, Liquid

Temperature Range
298.39 to 760.00 K

EQUATION 101

$$Y = \exp \left[A + \frac{B}{T} + C \ln T + DT^E \right]$$

Calculator
Temperature: 400
Value: 1398.435 Pa

Calculate

Coefficients

Units	Pa
A	124.1
B	-12250
C	-14.546
D	0.0000057497
E	2
Error	< 3%
Ave Dev	1.4
Max Dev	6.5
Data Type	Experimental
Date	7/31/1996
NotelD	

Temperature Range
From 298.39 to 760.00 with 20

☒ Points
☐ Increment

Reset Values

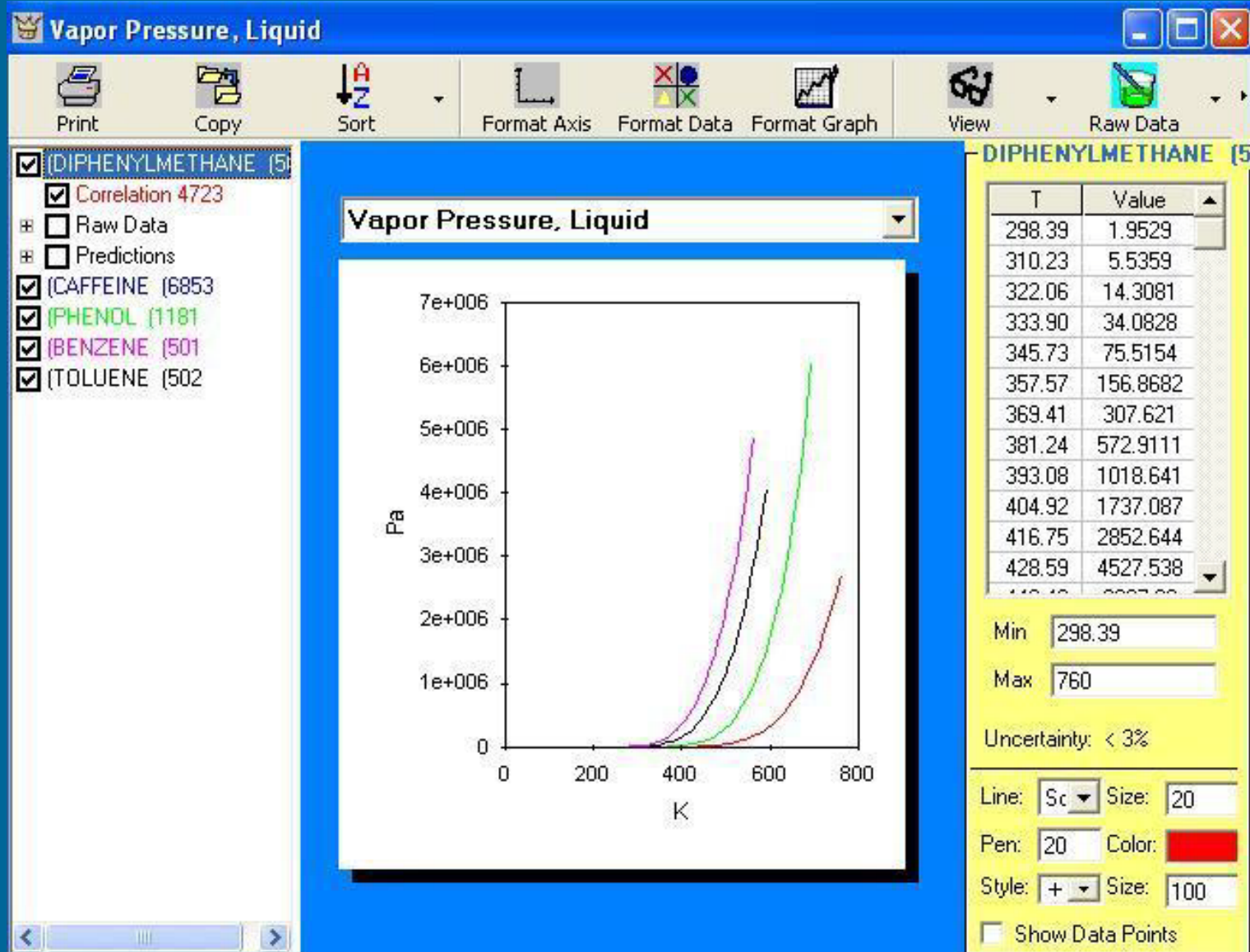
T/K	Pa
298.39	1.9529
322.69	15.0061
346.98	81.7936
371.28	340.4768
395.57	1143.582
419.87	3231.602
444.16	7935.398
468.46	1.7366E+04
492.75	3.4558E+04
517.05	6.3547E+04
541.34	1.0940E+05
565.64	1.7822E+05
589.93	2.7716E+05
614.23	4.1451E+05
638.52	5.9984E+05

Tabulate

Graph

Note:

Users can calculate temperature dependent property values at a specific temperature or over a range of temperatures.



Use DIADEM to simultaneously plot data for multiple compounds for any of the properties in the DIPPR® 801 database. Plots can simultaneously include correlations, raw data, and predicted values.

Database entry for ETHYL HYDROGEN SULFATE

Update New Import Delete Predict Print Check

General Constants T. Dependent Coefficients Add By Ref References/Notes

ChemID: 5894 Name: ETHYL HYDROGEN SULFATE

Retrieve

Constants

Constant Values

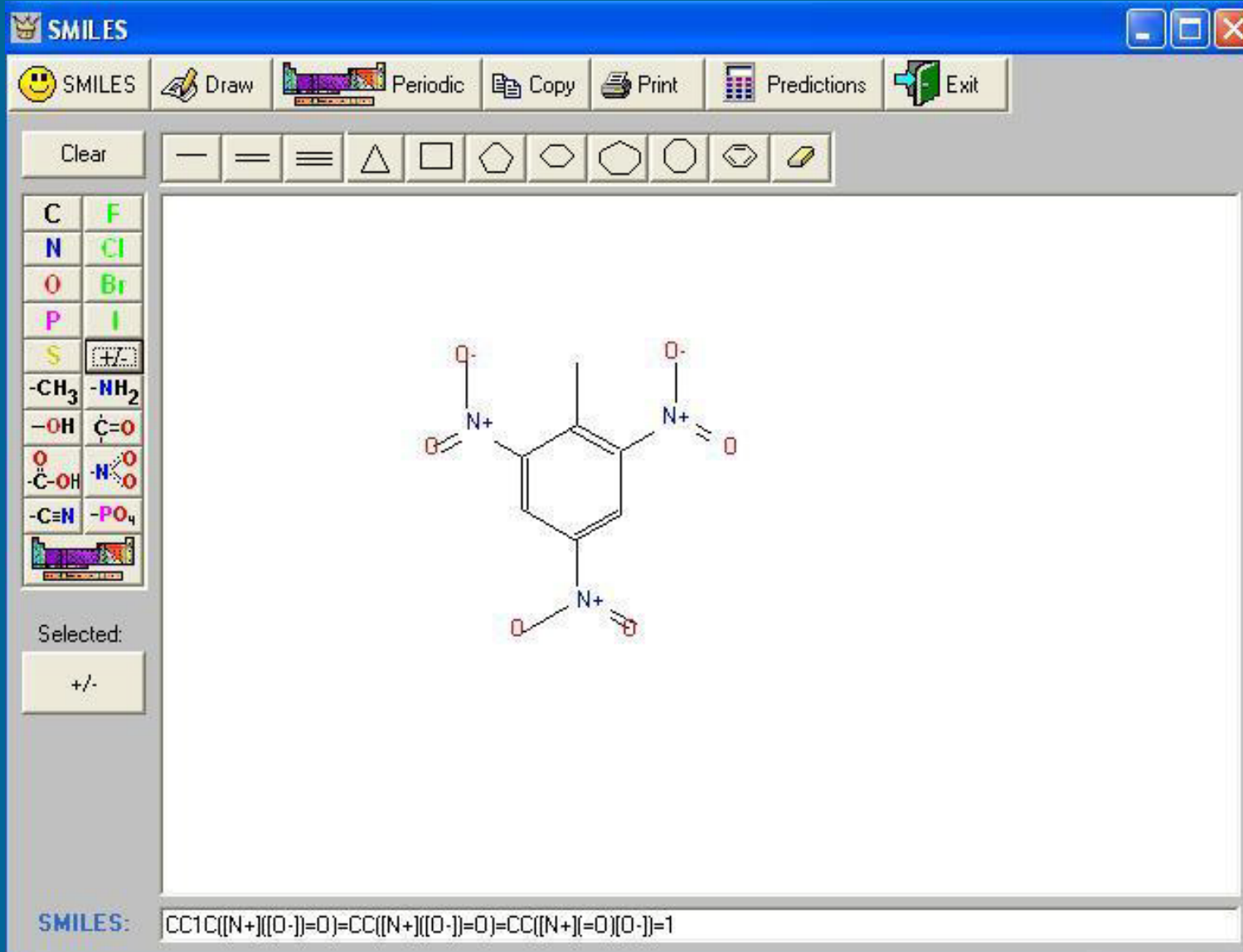
NBP	Value	Units	Deviation	Unknown	Accepted	10342	Unevaluated	Staff
HFOR	-8.0970E+08	J/kmol		Predicted	Accepted	9164	Staff	Staff
ENT	-6.6510E+08	J/kmol		Predicted	Accepted	13016	Staff	Staff
ENT		J/kmol-K						
HSTD	-8.8730E+08	J/kmol		Predicted	Accepted	13016	Staff	Staff
GSTD	-6.9800E+08	J/kmol		Defined	Accepted	13016	Staff	Staff
SSTD	2.1050E+05	J/kmol-K		Predicted	Accepted	13016	Staff	Staff
HFUS		J/kmol			Accepted			
HCOM	-9.2199E+08	J/kmol		Predicted	Accepted	13016	Staff	Staff
RG	0.493875			Defined	Accepted	13016	Staff	Staff
RG		m						
DM	2.7940E+04	(J/m ³) ^{1/2}		Predicted	Accepted	13016	Staff	Staff
DM		C-m						
AIT	7.9600E+08	m ² /kmol		Predicted	Accepted	12965	Staff	Staff

Given as Range Calculate Error Add Clear

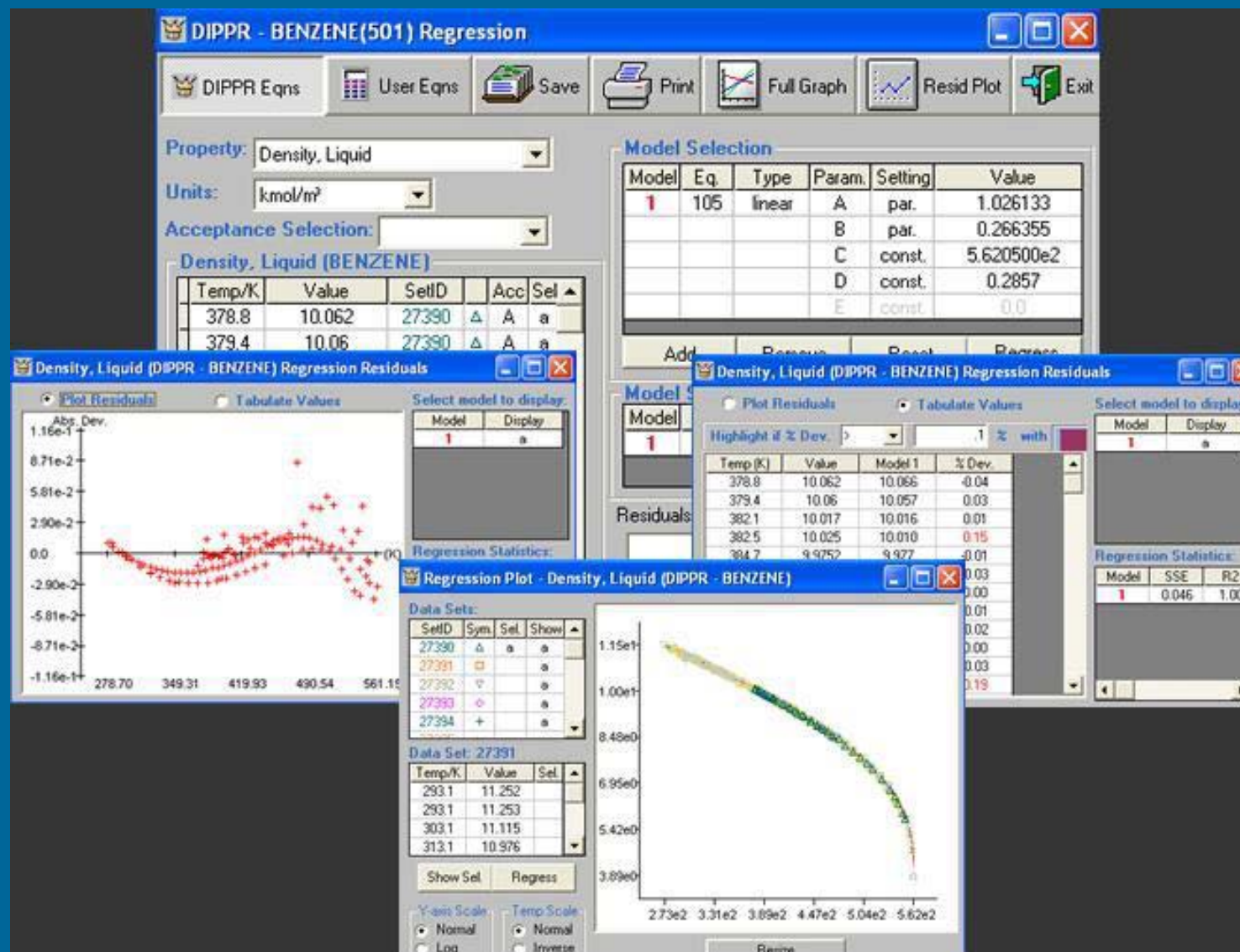
Note:

Update Exit

DIADEM enables users to create and maintain a database for user compounds and data. Then, the user's data can be easily compared to DIPPR® 801 data.



Draw a compound's structure and DIADEM will output a SMILES formula, or enter a SMILES formula and DIADEM will draw the structure.



DIADEM's regression package contains linear and nonlinear capabilities and allows regression of user equations. Data points used in the regression can be selected using the interactive regression graph. Residuals can be viewed in graphical or tabular form, with user-specified deviations highlighted.

1181 - PHENOL Constant Predictions

Calculate File Transfer Print Groups Evaluate Reset Multiple Constants T. Point

SMILES: c1ccccc1O

☒ Select by Property ☐ Select by Method

Critical Pressure

Acentric Factor
Autoignition Temperature
Critical Compressibility Factor
Critical Pressure
Critical Temperature
Critical Volume
Dielectric Constant
Dipole Moment
Flash Point
Heat of Combustion
Heat of Fusion at MP

☒ Ambrose - Original
☐ Ambrose - API
☒ Joback
☒ Lydersen
☐ Marrero-Pardillo
☒ Interpolation/Extrapolation (VP)
☐ Wilson-Jasperson
☐ Constantinou
☐ Shigaki
☐ Klincewicz-Reid
☐ Jalowka

Property Selection More

Property	Value	Method
MW	94.1112	Database
NBP	454.99	Database
TC	694.25	Database

Method	Value	Database	Units	Difference	% Dev
Ambrose - Original	6.1404E+06	6.1300E+06	Pa	1.0400E+04	0.17 %
Joback	5.9263E+06	6.1300E+06	Pa	-2.0370E+05	-3.32 %
Lydersen	6.1619E+06	6.1300E+06	Pa	3.1900E+04	0.52 %
Interpolation/Extrapolation (VP)	6.0585E+06	6.1300E+06	Pa	-7.1500E+04	-1.17 %
Nannoolal-PC	5.7548E+06	6.1300E+06	Pa	-3.7520E+05	-6.12 %

Ambrose - Original method predicting PC: Valid for most organic compounds including highly halogenated, aliphatics, aromatics, rings, and some silicon containing compounds.

Policies and Procedures:
PC (1) - Organic - Marrero-Pardillo - Inorganics - Extrapolate VP data to estimated TC (avoid other prediction methods)

DIADEM's prediction package allows users to select published predictive methods to estimate a properties for ANY compound, even those not included in the DIPPR® 801 database.