

AMProp_Calc

Version 0

User Guide

INSTALLATION

Before installing please read the License Agreement and agree to its terms and conditions.

To install expand the zipped file AMProp_Calc.zip in drive "C:". The folder AMProp_Calc and its content MUST BE in the root of drive C:

The folder **C:\AMProp_Calc** will be accessed by the Excel Add-in.

Add-in can be installed through the Excel Add-In manager or by opening directly the file "AMProp_Calc.xla." in the folder C:\AMProp_Calc

Note: The macros from this file must be enabled for the Add-in to function.

FUNCTIONS

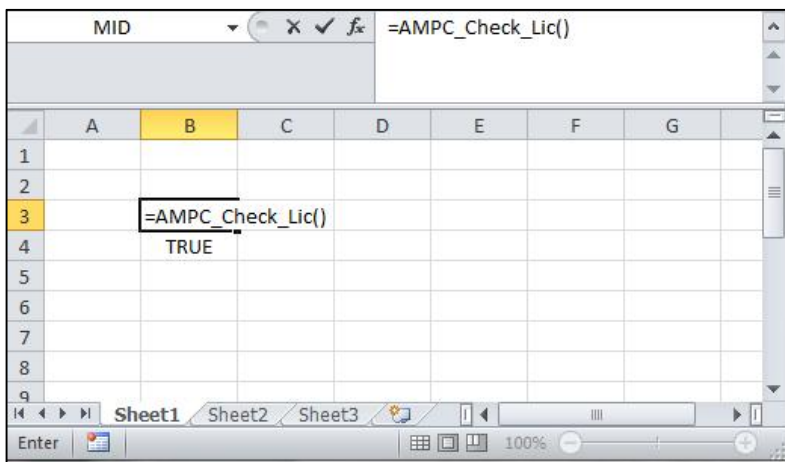
AMPC_Check_Lic()

Function required to be called within the Excel Sheet. This function will check the Validity of the License and activate the rest of function within the Add-in.

Returns:

True	If license IS VALID
False	If license IS NOT VALID or there are missing files to be used by the Add-in. The Add-in AMPro_Calc will not work. Contact the licensor to purchase or renew the license

Example:



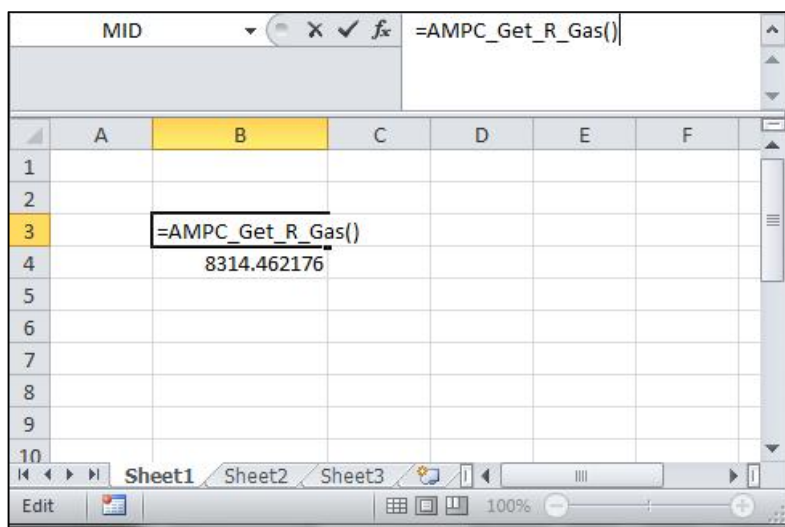
AMPC_Get_R_Gas()

Function returns the Ideal Gas Constant R

Returns:

8314.462176 Joule/(Kmol-K)

Example:



AMPC_Get_CompList()

Function returns the list of compound available in the AMProp_Calc library.

Returns:

An array containing:

Index	Value
1	Number of compounds in the Library
2 to Value of Index 1	Name of available compound

Note: The values are return column wise. In order to list the in Row wise the excel function "TRANSPOSE()" must be used to modify the orientation of the array

Example:

	A	B	C	D	E	F	G
1							
2		CompList()			54		
3		HYDROGEN			HYDROGEN		
4		METHANE			METHANE		
5		ACETYLENE			ACETYLENE		
6		ETHYLENE			ETHYLENE		
7		ETHANE			ETHANE		
8		PROPADIENE			PROPADIENE		
9							
10							

Note: To display the results in the various cells, select the range of cells (various rows) and after typing the formula =TRANSPOSE(AMPC_Get_ComplList()) press <CTRL> <SHIFT> <ENTER>

The range of cell will show the formula {=TRANSPOSE(AMPC_Get_ComplList())}

AMPC_Get_CASNO(CompName)

Function gets the CAS Registry Number. CAS Registry Number, is a unique numerical identifier assigned by Chemical Abstracts Service. Most of the functions in the Add-in use the CAS Number (instead of the Compound Name) to access the information required for property estimation.

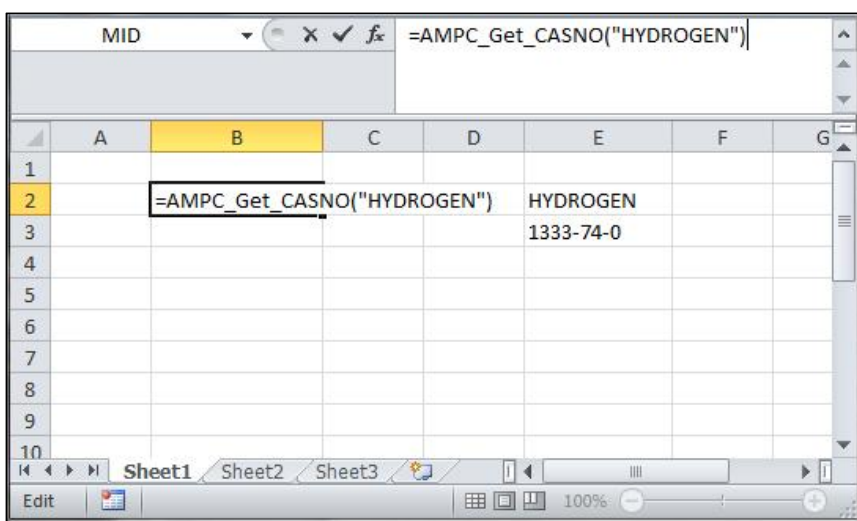
Input:

CompName: Name of the compound as appears in the available library. The Input can be the name of the compound in "", of a reference to a cell containing the name of the compound

Returns:

String containing the CAS Registry Number of the compound.

Example:



AMPC_Read_Pure_Info(CASNO)

The function reads the available information of the compound with CAS registry number CASNO in the library.

Input:

CASNO: The compound's CAS Number. The Input can be the name of the compound in “ ”, of a reference to a cell containing the name of the compound

Returns:

If CASNO is available in library function returns an array containing

Index	Value
1	MW: Molecular Weight
2	Tc: Critical Temperature in K
3	Pc: Critical Pressure in Pa
4	Vc: Critical Specific Volume in m3/Kmol
5	Tm: Melting Temperature in K
6	Hf: Enthalpy of formation in KJ/Kmol
7	Gibb free energy in KJ/Kmol
8	Entropy of Ideal gas @ 25oC and 1 atm in KJ/Kmol-K
9	LHV: Low Heat Value in KJ/Kmol
10	HHV: High Heat Value in KJ/Kmol
11	HComb: heat of combustion in KJ/Kmol
12	acenf (w) : Acentric factor

Otherwise returns an array of Zeros

Note: The values are return column wise. In order to list the in Row wise the excel function “TRANSPOSE()” must be used to modify the orientation of the array

Example:

	A	B	C	D	E	F	G
1	PROPANE				PROPANE		
2	74-98-6				74-98-6		
3		d_Pure_Info(B2))				44.09574	
4						369.83	
5						4247999.963	
6						0.2	
7						85.55	
8						-104679.9144	
9						-24390.0004	
10						270.2002096	
11						2043837.549	
12						2220000	
13						-2043104	
14						0.152291	
15							

Note: To display the results in the various cells, select the range of 12 cells (12 rows) and after typing the formula =TRANSPOSE(AMPC_Read_Pure_Info(B2)) press <CTRL> <SHIFT> <ENTER>

AMPC_Get_Pure_Property(CASNO, Prop)

The function gets a particular property for an available compound.

Input:

CASNO: String, CAS Registry number

Prop: String. Property to be get. The Value can be:

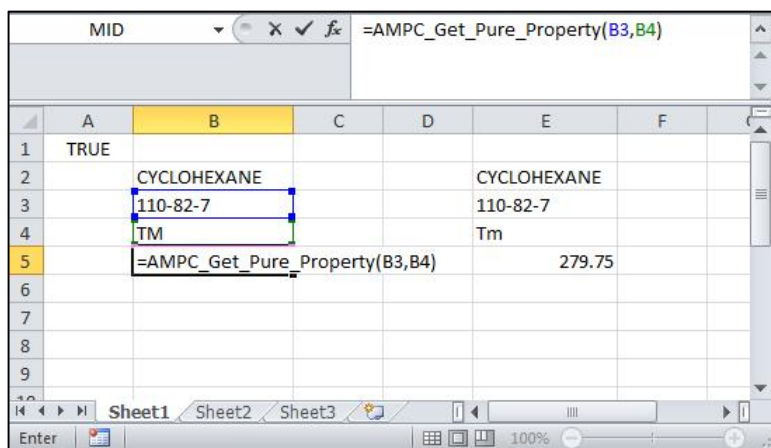
Prop	To Get
"MW"	Molecular Weight
"Tc"	Critical Temperature in K
"Pc"	Critical Pressure in Pa
"Vc"	Critical Specific Volume in m3/Kmol
"Tm"	Melting Temperature in K
"Hf"	Enthalpy of formation in KJ/Kmol
"Gf"	Gibb free energy in KJ/Kmol
"LHV"	Entropy of Ideal gas @ 25oC and 1 atm in KJ/Kmol-K
"HHV"	Low Heat Value in KJ/Kmol
"HComb"	High Heat Value in KJ/Kmol
"acenf"	heat of combustion in KJ/Kmol

Returns:

The value of the selected property

If CASNO or Prop are a not valid entry, returns Zero

Example:



	A	B	C	D	E	F
1	TRUE					
2		CYCLOHEXANE			CYCLOHEXANE	
3		110-82-7			110-82-7	
4		Tm			Tm	
5		=AMPC_Get_Pure_Property(B3,B4)			279.75	
6						
7						
8						
9						

AMPC_Pure_Z(w, Pr, Tr)

Calculates the Gas Compressibility Factor (Z)

Input:

w: Acentric Factor

Pr: Reduced Pressure ($Pr = P/P_c$)

Tr: Reduced Temperature ($Tr = T/T_c$)

Where P = Pressure, P_c = Critical Pressure, T = Temperature, T_c = Critical Temperature

w, P_c and T_c can be obtained using `AMPC_Get_Pure_Property(CASNO, Prop)` or `AMPC_Read_Pure_Info(CASNO)`

Returns:

The function returns an array of 3 elements

Index	Value
1	Compressibility Factor
2	Number of iteration made to achieve the solution
3	Value of the Converging Function (ideally Zero)

Note: If value of Index 2 is 100 the maximum iterations have been reached. Value of Z may not be correct.

The function can be used as an array or as a value. To display the results in the various cells, select the range of 3 cells (3 rows) and after typing the formula `=TRANSPOSE(AMPC_Read_Pure_Z(C9,C5,C8))` press <CTRL> <SHIFT> <ENTER>

Example:

E3		{=TRANSPOSE(AMPC_Pure_Z(C9,C5,C8))}						
	A	B	C	D	E	F	G	H
1	TRUE	NITROGEN						
2		CASNO	7727-37-9		Z as Array		Z as Value	
3		P	500000 Pa		1.000635141		1.0006351	
4		Pc	3400000.91 Pa		2			
5		Pr	0.14705878		1.30556E-12			
6		T	323.15 K					
7		Tc	126.2 K					
8		Tr	2.56061807					
9	w	acenf	0.0377215					
10								
11								
12								

AMPC_Pure_PSat(CASNO, T)

The function calculates the Vapor Pressure or the Saturation Pressure at a given temperature.

Input:

CASNO: String, CAS Registry number

T: Temperature in Kelvin (K)

Returns:

The function returns an array of 5 elements

Index	Value
1	Vapor Pressure in Pa
2	Value of the Equation of State at T and Psat (Ideally Zero)
3	Vapor Specific Volume @ T and Psat in m ³ /Kmol
4	Compressibility Factor (Z)
5	Number of Iterations to get the Z

T must be in the range $T_m < T < T_c$. If not Function returns Zero

T_m = Melting Temperature, T_c = Critical Temperature

Note: If value of Index 5 is 100 the maximum iterations have been reached. Value of Z may not be correct.

The function can be used as an array or as a value. To display the results in the various cells, select the range of 5 cells (5 rows) and after typing the formula
`=TRANSPOSE(AMPC_Pure_PSat(CASNO,T))` press <CTRL> <SHIFT> <ENTER>

Example:

E3		fx		{=TRANSPOSE(AMPC_Pure_PSat(B2,B5))}				
	A	B	C	D	E	F	G	H
1	TRUE	PROPANE			Psat As Array		Psat as Value	
2	CASNO	74-98-6					=AMPC_Pure_PSat(B2,B5)	
3	Tc	369.83 K		Psat	837489.2829		837489.28	
4	Tm	85.55 K		EOS	3.49246E-10			
5	T	293.15		V	2.463218635			
6				Z	0.846365903			
7				Z iter	5			
8								
9								
10								
11								

AMPC_Pure_TSat(CASNO, P)

The function calculates the Saturated Temperature at a given Pressure.

Input:

CASNO: String, CAS Registry number

P: Pressure in Pa

Returns:

The function returns an array of 6 elements

Index	Value
1	Saturation Temperature in Kelvin (K)
2	Number of Iteration to get the TSat
3	Value of the Equation of State at P and Tsat (Ideally Zero)
4	Vapor Specific Volume @ T and Psat in m ³ /Kmol
5	Compressibility Factor (Z)
6	Number of Iterations to get the Z

P must be in the range $P < P_c$. If not Function returns Zero

P_c = Critical Pressure

Note: If value of Index 2 or 6 is 100 the maximum iterations have been reached. Value of TSat or Z may not be correct.

The function can be used as an array or as a value. To display the results in the various cells, select the range of 6 cells (6 rows) and after typing the formula

=TRANSPOSE(AMPC_Pure_TSat(CASNO,T)) press <CTRL> <SHIFT> <ENTER>

Example:

AMPC_Pure_DHVapmol(CASNO, Tr)

The function calculates the specific molar Heat of Vaporization at a given Temperature

Input:

CASNO: String, CAS Registry number

Tr: Reduced Temperature

Returns:

The Heat of Vaporization in Joule/Kmol

Tr must be in the range $Tr < 1$. If not Function returns Zero

Tr = Reduced Temperature, $Tr = T/T_c$; T_c = Critical Temperature

Example:

D4		fx		=AMPC_Pure_DHVapmol(B2,B5)		
	A	B	C	D	E	F
1	TRUE	TOLUENE				
2	CASNO	108-88-3				
3	Tc	591.75 K				
4	T	330 K		36388569.25 J/Kmol		
5	Tr	0.5576679				
6						
7						
8						

AMPC_Pure_LiqMolCp(CASNO, T)

The function calculates the specific molar Calorific Value for liquid phase at constant Pressure (Cp) at a given Temperature

Input:

CASNO: String, CAS Registry number

T: Temperature in Kelvin (K)

Returns:

The Liquid molar Calorific Value (Cp) in Joule/Kmol-K

T must be in the range $T_m < T < T_c$. If not Function returns Zero

Example:

AMPC_Pure_VapMolCp(CASNO, T)

Input:

Returns:

Example:

	A	B	C	D	E	F	G
1	TRUE						
2			ETHANE				
3		CASNO	74-84-0				
4		T	303.15 K				
5							
6			53022.27774	J/kmol-K			
7							
8							

AMPC_Pure_LiqVis(CASNO, T)

The function calculates the Dynamic Viscosity of a liquid at a given Temperature

Input:

CASNO: String, CAS Registry number

T: Temperature in Kelvin (K)

Returns:

The Liquid Dynamic Viscosity in Pa.s

T must be in the range $T_m < T < T_c$. If not Function returns Zero

T_m = Melting Temperature, T_c = Critical Temperature

Example:

C6		fx		=AMPC_Pure_LiqVis(C3,C4)			
	A	B	C	D	E	F	G
1	TRUE						
2			WATER				
3		CASNO	7732-18-5				
4		T	293.15 K				
5							
6			0.001021406	Pa.s			
7			1.021405658	cp			
8							

AMPC_Pure_GasVis(CASNO, T)

The function calculates the Dynamic Viscosity of gas or vapor at a given Temperature

Input:

CASNO: String, CAS Registry number

T: Temperature in Kelvin (K)

Returns:

The Dynamic Viscosity Pa.s

Example:

C6		fx		=AMPC_Pure_LiqVis(C3,C4)			
	A	B	C	D	E	F	G
1	TRUE						
2			WATER				
3		CASNO	7732-18-5				
4		T	423.15 K				
5							
6			0.000179488	Pa.s			
7			0.179487738	cp			
8							

AMPC_Pure_State(CASNO, P, T)

The function finds the state of a compound at a given Pressure and Temperature

Input:

CASNO: String, CAS Registry number

P: Pressure in Pa

T: Temperature in Kelvin (K)

Returns:

Value	Condition
1	Solid
2	Liquid
3	Liquid – Vapor Equilibrium
4	Vapor
5	Gas
6	Super Critical

Example:

C7		fx		=AMPC_Pure_State(C3,C4,C5)			
	A	B	C	D	E	F	
1	TRUE						
2			CYCLOHEXANE	WATER			
3		CASNO	110-82-7	7732-18-5			
4		P	101235	101235 Pa			
5		T	263.15	373.15 K			
6							
7			1	3			
8							
9							

AMPC_Pure_Enthalpy(CASNO, P, T)

Calculates the specific molar Enthalpy (H) at a given Pressure and Temperature

Input:

CASNO: String, CAS Registry number

P: Pressure in Pa

T: Temperature in Kelvin (K)

Returns:

The specific molar Enthalpy in J/Kmol

As reference H = 0 for ideal gas at 1amt and 25 oC.

Example:

C8		=AMPC_Pure_Enthalpy(C3,C4,C5)						
	A	B	C	D	E	F	G	
1	TRUE							
2			ETHYLENE					
3		CASNO	74-85-1					
4		P	2026500 Pa					
5		T	250 K					
6		Tc	282.34 K					
7		Tsat	244.842188 K					
8		H (T)	-3435315.5 J/Kmol					
9		H(Tsat+0.01)	-3719857 J/Kmol	DH		-284541 J/Kmol		
10		H(Tsat-0.01)	-12742949 J/Kmol	DH		-9023092 J/Kmol		
11						-9307633		
12								
13		-DHVap	-9021626.5 J/Kmol			1465.021		
14						-0.016%		

AMPC_Pure_Entropy(CASNO, P, T)

Calculates the specific molar Entropy (S) at a given Pressure and Temperature

Input:

CASNO: String, CAS Registry number

P: Pressure in Pa

T: Temperature in Kelvin (K)

Returns:

The specific molar Entropy in J/Kmol-K

As reference $S = 0$ for ideal gas at 1amt and 25 oC.

Example:

C7		fx		=AMPC_Pure_Entropy(C3,C4,C5)			
	A	B	C	D	E	F	G
1	TRUE						
2			METHANE				
3		CASNO	74-82-8				
4		P	2026500 Pa				
5		T	250 K				
6		Tc	190.564 K				
7		Entropy	-7477.4753 J/Kmol-K				
8							
9		P2	4053000 Pa				
10		T2 (S1=S2)	258.978156 K				
11		Entropy	-7477.4753 J/Kmol-K				
12		S1-S2	4.3923E-08 J/Kmol-K				
13							

AMPC_Read_ComputerInfo()

Function reads information from the host local computer

Returns:

Returns an array with 4 elements containing the following information

Index	Description
1	Computer Name
2	Manufacturer
3	Model
4	Serial Number

This information will be required by Licensor to issue a valid license

The function must be entered as an array. To display the results in the various cells, select the range of 4 cells (4 rows) and after typing the formula =TRANSPOSE(AMPC_Read_ComputerInfo()) press <CTRL> <SHIFT> <ENTER>

Example:

	B3		f_x {=TRANSPOSE(AMPC_Read_ComputerInfo())}					
	A	B	C	D	E	F	G	H
1	TRUE							
2								
3		JKTMICHINIE-TH						
4		LENOVO						
5		20AMA0LDID						
6		PF00B8XT						
7								
8								