

# **Property Library for Combustion Gas Mixtures calculated from VDI-Guideline 4670**

## **LibIDGAS**

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# Property Functions of LibIDGAS

## 1. Range of Validity and Structure of the Program Library

The thermodynamic properties of combustion gas mixtures in the ideal gas state are calculated corresponding to the

VDI Guideline 4670 [21].

The transport properties are calculated corresponding to

*Brandt* [15] and VDI-Wärmeatlas [19].

Important property constants were taken from the compendium from *Blanke* [20].

The mixture can contain the following components:

Number	Component	
1	Argon	Ar
2	Neon	Ne
3	Nitrogen	N <sub>2</sub>
4	Oxygen	O <sub>2</sub>
5	Carbon monoxide	CO
6	Carbon dioxide	CO <sub>2</sub>
7	Steam	H <sub>2</sub> O
8	Sulfur dioxide	SO <sub>2</sub>
9	Air (dry)	
10	Air nitrogen	

### Range of validity:

Temperature  $t$ : from -73.15 °C to 3026.85 °C

Mixture pressure  $p$ : from > 0 bar to 10 (30), max 50 bar

The pressure range is limited for gases and mixtures in the ideal gas state.

For temperatures above 1000 °C and mole fractions of oxygen of more than 1 % ( $\psi_{O_2} \geq 0.01$ ) the dissociation based on the VDI 4670 for the gases nitrogen, oxygen, carbon dioxide, steam, and sulfur dioxide are considered. For programming reasons, the calculation of the correction for the dissociation is already carried out from 500 °C.

## 2. Property Functions for Ideal Gas Mixtures

Functional Dependence	Function Name	Call as Fortran Program	Property or Function	Unit of the Result	Reference	Page
$a = f(p, t, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	a_pt_id	a_pt_id(p,t,type,zu(1:10))	Thermal diffusivity	m <sup>2</sup> /s	[15], [18]	3/1
$c_p = f(p, t, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	cp_pt_id	cp_pt_id(p,t,type,zu(1:10))	Specific isobaric heat capacity	kJ/(kg · K)	[18]	3/2
$c_v = f(p, t, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	cv_pt_id	cv_pt_id(p,t,type,zu(1:10))	Specific isochoric heat capacity	kJ/(kg · K)	[18]	3/3
$\eta = f(t, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	Eta_t_id	Eta_t_id(t,type,zu(1:10))	Dynamic viscosity	Pa·s = kg/(m·s)	[15], [18]	3/4
$h = f(p, t, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	h_pt_id	h_pt_id(p,t,type,zu(1:10))	Specific enthalpy	kJ/kg	[18]	3/5
$\kappa = f(p, t, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	Kappa_pt_id	Kappa_pt_id(p,t,type,zu(1:10))	Isentropic exponent		[18]	3/6
$\lambda = f(t, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	Lambda_t_id	Lambda_t_id(t,type,zu(1:10))	Thermal conductivity	W/(m · K)	[15]	3/7
$M = f(\xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	M_id	M_id(type,zu(1:10))	Molar mass of the mixture	kg/kmol	[17]	3/8
$\nu = f(p, t, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	Ny_pt_id	Ny_pt_id(p,t,type,zu(1:10))	Kinematic Viscosity	m <sup>2</sup> /s	[15], [16]	3/9
$p = f(t, s, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	p_ts_id	p_ts_id(t,s,type,zu(1:10))	Backward Function: Mixture pressure from temperature and entropy of the mixture	bar	[18]	3/10
$p = f(t, v, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	p_tv_id	p_tv_id(t,v,type,zu(1:10))	Backward Function Mixture pressure from temperature and specific volume	bar	Ideal gas equation	3/11
$Pr = f(p, t, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	Pr_pt_id	Pr_pt_id(p,t,type,zu(1:10))	<i>Prandtl</i> -number		[15], [16]	3/12
$\psi_i = f(i, \xi_1 \dots \xi_{10})$	Psi_igas_Xsi_id	Psi_igas_Xsi_id(i,Xsi(1:10))	Mole fraction of the mixture gas i from the mass fractions of all mixture gases	kmol/kmol	Mixture calculation	3/13
$R = f(\xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	R_id	R_id(type,zu(1:10))	Specific gas constant	kJ/(kg · K)	[17]	3/14
$\rho = f(p, t, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	Rho_pt_id	Rho_pt_id(p,t,type,zu(1:10))	Density	kg/m <sup>3</sup>	Ideal gas equation	3/15

Functional Dependence	Function Name	Call as Fortran Program	Property or Function	Unit of the Result	Reference	Page
$s = f(p, t, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	s_pt_id	s_pt_id(p,t,type,zu(1:10))	Specific entropy of the mixture	kJ/(kg · K)	[18]	3/16
$t = f(p, h, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	t_ph_id	t_ph_id(p,h,type,zu(1:10))	Backward Function: Temperature from pressure and enthalpy of the mixture	°C	[18]	3/17
$t = f(p, s, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	t_ps_id	t_ps_id(p,s,type,zu(1:10))	Backward Function: Temperature from pressure and entropy of the mixture	°C	[18]	3/18
$t = f(p, v, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	t_pv_id	t_pv_id(p,v,type,zu(1:10))	Backward Function: Temperature from pressure and specific volume of the mixture	°C	[18]	3/19
$u = f(p, t, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	u_pt_id	u_pt_id(p,t,type,zu(1:10))	Specific internal energy	kJ/kg		3/20
$v = f(p, t, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	v_pt_id	v_pt_id(p,t,type,zu(1:10))	Specific volume	m <sup>3</sup> /kg	Ideal gas equation	3/21
$w = f(p, t, \xi_1 \dots \xi_{10} \text{ or } \psi_1 \dots \psi_{10})$	w_pt_id	w_pt_id(p,t,type,zu(1:10))	Isentropic speed of sound of the mixture	m/s	[18]	3/22
$\xi_i = f(i, \psi_1 \dots \psi_{10})$	Xsi_igas_Psi_id	Xsi_igas_Psi_id(i,Psi(1:10))	Mass fraction of the mixture gas i from the mole fractions of all mixture gases	kg/kg	Mixture calculation	3/23

## Units:

Symbol	Name	Unit
t	Temperature	°C
p	Mixture pressure	bar
$\xi_1 \dots \xi_{10}$	Mass fractions of the components	kg/kg
$\psi_1 \dots \psi_{10}$	Mole fractions, volume fractions of the components	kmol/kmol
type	Input: type = 1 for mass fractions $\xi_1, \dots, \xi_{10}$ type = 0 for mole fractions $\psi_1, \dots, \psi_{10}$	
comp(1:10) for type =1	Mass fractions $\xi_1, \dots, \xi_{10}$	kg/kg
comp(1:10) for type =0	Mole fractions $\psi_1, \dots, \psi_{10}$	kmol/kmol

## Mixture Gases:

Gas	Mixture gas	
1	Argon	Ar
2	Neon	Ne
3	Nitrogen	N <sub>2</sub>
4	Oxygen	O <sub>2</sub>
5	Carbon monoxide	CO
6	Carbon dioxide	CO <sub>2</sub>
7	Steam	H <sub>2</sub> O
8	Sulfur dioxide	SO <sub>2</sub>
9	Air (dry) from VDI4670 [21]	Composition in mole fractions: 78.1109 % N <sub>2</sub> 20.9548 % O <sub>2</sub> 0.9343 % Ar Composition in mass fractions: 75.5577 % N <sub>2</sub> 23.1535 % O <sub>2</sub> , 1.2888 % Ar
10	Air nitrogen from <i>Brandt</i> [15]	Composition in mole fractions: 98.8180 % N <sub>2</sub> 1.1820 % Ar Composition in mass fractions: 98.3229 % N <sub>2</sub> 1.6771 % Ar

### Range of Validity:

Temperature:	t = -73.15 °C ... 3026.85 °C
Pressure:	p = 0.01 mbar ... 50 bar

### Reference States:

Property	Gases (except steam)	Steam
Pressure	1.01325 bar	0.006112127 bar
Temperature	0.0 °C	0 °C
Enthalpy	0 kJ/kg	2500.9342 kJ/kg
Entropy	0 kJ/kg K	9.15591 kJ/(kg K)

### Variable Types for Function Call:

All functions:	Double
Variable p, t, v, h, s :	Double
Variable to [1..10] :	Array of Double
Variable type, i :	Integer

### Note:

If the input values are located outside the range of validity or if they do not fit together, the chosen function to be calculated results in -1.