



Materials Report

Workspace: ACL_Navarra_Nov2024_8.71

Material: ACETYLENE

ACL_Navarra_Nov2024_8.71\Physical Properties System\Materials\ACETYLENE

Property method template	PhastMC
DIPPR version	2018

General

Constants

Acentric factor	0,191185	
Aerosol class number	2	
Critical pressure	61,38	bar
Critical temperature	35,15	degC
Flammable/Toxic flag	Flammable	
Melting point	-80,75	degC
Molecular weight	26,0373	
Normal boiling point	-84,15	degC
Reactivity with atmosphere	Not Strongly Reactive	
SRK alpha calculation flag	Soave	
Triple point pressure	1,27445	bar
Triple point temperature	-80,75	degC
Carbon hydrogen ratio	1	
Solid Phase Modelling Enabled (CO2 Only)	No	
Enthalpy of Fusion at Melting Point	3770	kJ/kg

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Heat of vapourisation	106	1,7059E+07	-0,52025	1,0982	-0,29832	0	-80,75	35,15	1	Constant value above fraction Tc

Flammable

Constants

Combustion at	1,04032	
Combustion ct	0,0775194	
Emissive power length scale		m
Flash point	-122,15	degC

Heat of combustion	1,257E+06	kJ/kmol
Immediate ignition category	High	
Laminar burning velocity	1,55	m/s
Lower flammability limit	25000	ppm
Luminous/Smoky flame flag	General	
Maximum burn rate	0	kg/m2.s
Maximum surface emissive power		kW/m2
Pool fire burn rate length	0	m
TNT explosion efficiency	0	%
Upper flammability limit	800000	ppm

Toxic Constants

Dangerous dose 2		
Dangerous dose 3		
Dangerous dose 4		
Dangerous dose 5		
Dangerous dose 6		
Dangerous toxic load Note: Units are concentration in ppm and time in minutes		
ERPG 1		ppm
ERPG 2		ppm
ERPG 3		ppm
IDLH concentration		ppm
STEL concentration		ppm
Toxic property A	0	
Toxic property B	0	
Toxic property N	0	

Transport Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Liquid thermal conductivity	100	0,33363	-0,00083655	0	0	0	-80,75	-23,15	1	Constant value above fraction Tc
Liquid viscosity	101	6,224	-151,8	-2,6554	0	0	-80	-6,10352E-06	1	Constant value above fraction Tc

Surface tension	106	0,061441	1,1972	0	0	0	-90	35,15	1	Constant value above fraction Tc
Vapour thermal conductivity	102	7,5782E-05	1,0327	-36,227	31432		-83,8	726,85	1	None (use equation)
Vapour viscosity	102	1,2025E-06	0,4952	291,4	0		-80,75	326,85	1	None (use equation)

Heat capacity Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Ideal gas heat capacity	127	33257,9	7,11015E+07	1601,77	-7,10776E+07	1602,12	-253,15	1226,85	1	None (use equation)
Liquid heat capacity	100	-122020	3082,7	-15,895	0,027732	0	-80,75	-23,15	1	None (use equation)

Vapour pressure Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Vapour pressure	101	39,63	-2552,2	-2,78	2,393E-16	6	-80,75	35,15	1	Vapour Pressure Extrapolation

Density Coefficients

Name	Equation	A	B	C	D	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Saturated liquid density	105	2,4507	0,27448	308,3	0,28752	-80,75	35,15	1	Constant value above fraction Tc

Virial Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Second virial equation coefficient	104	0,0315	-4,59	-5,04E+06	1,083E+18	-1,583E+20	-118,99	1268,5	1	None (use equation)

Association Constants

Acid association flag	Not Modelled	
Enthalpy interpolation range	0	delC

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Dimer coefficients	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)
Hexamer coefficients	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)
Octamer coefficients	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)
Trimer coefficients	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)

Water Constants

Heat of solution	0	kJ/kg
Liquid water enthalpy coefficient A	0	
Liquid water enthalpy coefficient B	0	
Liquid water enthalpy coefficient C	0	
Liquid water enthalpy coefficient D	0	
Liquid water surface tension	0	N/m
Reaction with water model	None	



Solubility in water	0	
Water heat transfer coefficient	500	W/m2.degK



Material: HYDROGEN FLUORIDE

ACL_Navarra_Nov2024_8.71\Physical Properties System\Materials\HYDROGEN FLUORIDE

Property method template	PhastMC
DIPPR version	2018

General Constants

Acentric factor	0,382283	
Aerosol class number	1	
Critical pressure	64,8	bar
Critical temperature	188	degC
Flammable/Toxic flag	Toxic	
Melting point	-83,36	degC
Molecular weight	20,0063	
Normal boiling point	19,52	degC
Reactivity with atmosphere	HF Only	
SRK alpha calculation flag	Soave	
Triple point pressure	0,00336833	bar
Triple point temperature	-83,36	degC
Carbon hydrogen ratio	0	
Solid Phase Modelling Enabled (CO2 Only)	No	
Enthalpy of Fusion at Melting Point	4580,4	kJ/kg

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Heat of vapourisation	106	1,3451E+08	13,36	- 23,383	10,785	0 4,41		188	1	Constant value above fraction Tc

Flammable Constants

Combustion at	1	
Combustion ct	1	
Emissive power length scale	0	m
Flash point		degC
Heat of combustion	152400	kJ/kmol
Immediate ignition category	Unknown	

Laminar burning velocity		m/s
Lower flammability limit	-9,95E+40	ppm
Luminous/Smoky flame flag	Non-flammable	
Maximum burn rate	0	kg/m2.s
Maximum surface emissive power	0	kW/m2
Pool fire burn rate length	0	m
TNT explosion efficiency	0	%
Upper flammability limit	-9,95E+40	ppm

Toxic Constants

Dangerous dose 2	1440	
Dangerous dose 3	2640	
Dangerous dose 4		
Dangerous dose 5		
Dangerous dose 6		
Dangerous toxic load Note: Units are concentration in ppm and time in minutes	60	
ERPG 1	2	ppm
ERPG 2	20	ppm
ERPG 3	50	ppm
IDLH concentration		ppm
STEL concentration		ppm
Toxic property A	-8,62	
Toxic property B	1	
Toxic property N	1	

Transport Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Liquid thermal conductivity	100	0,7516	-	0	0	0	-83,36	121,3	1	Constant value above fraction Tc
Liquid viscosity	101	353,99	13928	-	-2962	-	-83,36	95,77	1	Constant value above fraction Tc
			0,0010874	41,717	0,5					

Surface tension	106	0,03648	1,4122	0	0	0	-83,36	188	1	Constant value above fraction Tc
Vapour thermal conductivity	102	3,4629E-05	1,1224	18,744	0		76,85	176,85	1	None (use equation)
Vapour viscosity	102	4,5101E-14	3,0005	-	521,83	76111	12,35	199,53	1	None (use equation)

Heat capacity Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Ideal gas heat capacity	107	29134	9325,2	2905	195	1326	-223,15	1226,85	1	None (use equation)
Liquid heat capacity	100	62520	-223,02	0,6297	0	0	-83,36	19,52	1	None (use equation)

Vapour pressure Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Vapour pressure	101	59,544	-	-	1,4161E-2	05	-83,36	188	1	Vapour Pressure Extrapolation

Density Coefficients

Name	Equation	A	B	C	D	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Saturated liquid density	105	2,8061	0,19362	461,15	0,29847	-83,36	188	1	Constant value above fraction Tc

Virial

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Second virial equation coefficient	100	0	0	0	0	0	-273,15	-273,15	1	None (use equation)

Association Constants

Acid association flag	Modelled	
Enthalpy interpolation range	30	delC

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Dimer coefficients	101	-21,83	3421,9	0	0	0	-273,15	-273,15	1	None (use equation)
Hexamer coefficients	101	-119,7	20130	0	0	0	-273,15	-273,15	1	None (use equation)
Octamer coefficients	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)
Trimer coefficients	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)

Water Constants

Heat of solution	3076	kJ/kg
Liquid water enthalpy coefficient A	0	
Liquid water enthalpy coefficient B	0	
Liquid water enthalpy coefficient C	0	
Liquid water enthalpy coefficient D	0	
Liquid water surface tension	0	N/m
Reaction with water model	None	
Solubility in water	1	
Water heat transfer coefficient	500	W/m2.degK



Material: NITRIC ACID

ACL_Navarra_Nov2024_8.71\Physical Properties System\Materials\NITRIC ACID

Property method template	PhastMC
DIPPR version	2018

General Constants

Acentric factor	0,714406	
Aerosol class number	1	
Critical pressure	68,901	bar
Critical temperature	246,85	degC
Flammable/Toxic flag	Toxic	
Melting point	-41,6	degC
Molecular weight	63,0128	
Normal boiling point	83	degC
Reactivity with atmosphere	Not Strongly Reactive	
SRK alpha calculation flag	Soave	
Triple point pressure	0,000607682	bar
Triple point temperature	-41,6	degC
Carbon hydrogen ratio	0	
Solid Phase Modelling Enabled (CO2 Only)	No	
Enthalpy of Fusion at Melting Point	10470	kJ/kg

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Heat of vapourisation	106	7,06042E+07	0,692931	0	0	0	-41,6	86	1	Constant value above fraction Tc

Flammable Constants

Combustion at	1	
Combustion ct	1	
Emissive power length scale	0	m
Flash point		degC
Heat of combustion	13400	kJ/kmol
Immediate ignition category	Unknown	

Laminar burning velocity		m/s
Lower flammability limit	-9,95E+40	ppm
Luminous/Smoky flame flag	Non-flammable	
Maximum burn rate	0	kg/m2.s
Maximum surface emissive power	0	kW/m2
Pool fire burn rate length	0	m
TNT explosion efficiency	0	%
Upper flammability limit	-9,95E+40	ppm

Toxic Constants

Dangerous dose 2	1440	
Dangerous dose 3	5520	
Dangerous dose 4		
Dangerous dose 5		
Dangerous dose 6		
Dangerous toxic load Note: Units are concentration in ppm and time in minutes	9,6	
ERPG 1	1	ppm
ERPG 2	6	ppm
ERPG 3	78	ppm
IDLH concentration		ppm
STEL concentration		ppm
Toxic property A	-18,6	
Toxic property B	1	
Toxic property N	1	

Transport Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Liquid thermal conductivity	100	0,12107	0,0005383	0	0	0	-40	160	1	Constant value above fraction Tc
Liquid viscosity	101	-28,886	1940	2,678	0	0	-6,10352E-06	94,75	1	Constant value above fraction Tc

Surface tension	100	0,08343	-0,0001455	0	0	0	-6,10352E-06	40	1	Constant value above fraction Tc
Vapour thermal conductivity	102	0,00063365	0,72057	645,24	0	83		726,85	1	None (use equation)
Vapour viscosity	102	2,2234E-07	0,72283	140,72	0	-41,6		726,85	1	None (use equation)

Heat capacity Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Ideal gas heat capacity	107	33440	70500	1041	44700	473	-173,15	1226,85	1	None (use equation)
Liquid heat capacity	100	131250	-121,9	0,1704	0	0	-34,58	29,74	1	None (use equation)

Vapour pressure Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Vapour pressure	101	170,14	-10078	-22,769	2,73E-05	2	-41,6	102,95	1	Vapour Pressure Extrapolation

Density Coefficients

Name	Equation	A	B	C	D	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Saturated liquid density	105	1,5895	0,2304	520	0,1933	-41,6	100	1	Constant value above fraction Tc

Virial

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Second virial equation coefficient	100	0	0	0	0	0	-273,15	-273,15	1	None (use equation)

Association Constants

Acid association flag	Not Modelled	
Enthalpy interpolation range	0	delC

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Dimer coefficients	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)
Hexamer coefficients	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)
Octamer coefficients	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)
Trimer coefficients	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)

Water Constants

Heat of solution	0	kJ/kg
Liquid water enthalpy coefficient A	0	
Liquid water enthalpy coefficient B	0	
Liquid water enthalpy coefficient C	0	
Liquid water enthalpy coefficient D	0	
Liquid water surface tension	0	N/m
Reaction with water model	None	
Solubility in water	0	
Water heat transfer coefficient	500	W/m2.degK



Material: AMMONIA

ACL_Navarra_Nov2024_8.71\Physical Properties System\Materials\AMMONIA

Property method template	PhastMC
DIPPR version	2018

General Constants

Acentric factor	0,252608	
Aerosol class number	1	
Critical pressure	112,8	bar
Critical temperature	132,5	degC
Flammable/Toxic flag	Both	
Melting point	-77,74	degC
Molecular weight	17,0305	
Normal boiling point	-33,43	degC
Reactivity with atmosphere	Not Strongly Reactive	
SRK alpha calculation flag	Soave	
Triple point pressure	0,0611109	bar
Triple point temperature	-77,74	degC
Carbon hydrogen ratio	0	
Solid Phase Modelling Enabled (CO2 Only)	No	
Enthalpy of Fusion at Melting Point	5657	kJ/kg

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Heat of vapourisation	106	3,1523E+07	0,3914	-0,2289	0,2309	0	-77,74	132,5	1	Constant value above fraction Tc

Flammable Constants

Combustion at	0,965278	
Combustion ct	0,143885	
Emissive power length scale	2,75	m
Flash point	-64,15	degC
Heat of combustion	316830	kJ/kmol
Immediate ignition category	Low	

Laminar burning velocity	0,45	m/s
Lower flammability limit	150000	ppm
Luminous/Smoky flame flag	General	
Maximum burn rate	0	kg/m2.s
Maximum surface emissive power	170	kW/m2
Pool fire burn rate length	0	m
TNT explosion efficiency	0	%
Upper flammability limit	280000	ppm

Toxic Constants

Dangerous dose 2	9600	
Dangerous dose 3	66000	
Dangerous dose 4		
Dangerous dose 5		
Dangerous dose 6		
Dangerous toxic load Note: Units are concentration in ppm and time in minutes	1800	
ERPG 1	25	ppm
ERPG 2	150	ppm
ERPG 3	750	ppm
IDLH concentration		ppm
STEL concentration		ppm
Toxic property A	-16,21	
Toxic property B	1	
Toxic property N	1	

Transport Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Liquid thermal conductivity	100	1,169	-0,002314	0	0	0	-77,74	126,9	1	Constant value above fraction Tc
Liquid viscosity	101	-6,743	598,3	-0,7341	-3,69E-27	10	-77,74	120	1	Constant value above fraction Tc

Surface tension	106	0,09051	1,0905	0	0	0	-77,74	132,5	1	Constant value above fraction Tc
Vapour thermal conductivity	102	9,6608E-06	1,3799	0	0		-73,15	626,85	1	None (use equation)
Vapour viscosity	102	4,1855E-08	0,9806	30,8	0		-77,74	726,85	1	None (use equation)

Heat capacity Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Ideal gas heat capacity	107	33427	48980	2036	22560	882	-173,15	1226,85	1	None (use equation)
Liquid heat capacity	114	61,289	80925	799,4	-2651	0	-70	128	1	None (use equation)

Vapour pressure Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Vapour pressure	101	90,483	-4669,7	-11,607	0,017194	1	-77,74	132,5	1	Vapour Pressure Extrapolation

Density Coefficients

Name	Equation	A	B	C	D	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Saturated liquid density	105	3,5383	0,25443	405,65	0,2888	-77,74	132,5	1	Constant value above fraction Tc

Virial

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Second virial equation coefficient	104	0,015	-19,9	-4,931E+06	-2,85E+18	4,434E+20	-73,15	426,85	1	None (use equation)

Association Constants

Acid association flag	Not Modelled
Enthalpy interpolation range	0 delC

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature [degC]	Maximum temperature [degC]	Fraction of critical temperature [fraction]	Supercritical extrapolation
Dimer coefficients	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)
Hexamer coefficients	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)
Octamer coefficients	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)
Trimer coefficients	101	0	0	0	0	0	-273,15	-273,15	1	None (use equation)

Water Constants

Heat of solution	540	kJ/kg
Liquid water enthalpy coefficient A	7,35583E+06	
Liquid water enthalpy coefficient B	-3,99268E+07	
Liquid water enthalpy coefficient C	3,3452E+07	
Liquid water enthalpy coefficient D	-3,45507E+06	
Liquid water surface tension	0	N/m



Reaction with water model	Raj & Reid	
Solubility in water	0,53	
Water heat transfer coefficient	200	W/m2.degK