

Materials Report

Workspace: CONSEQUENCE MODEL_16FEB2021

Material: 1,2-DICHLOROETHANE

CONSEQUENCE MODEL_16FEB2021\Physical Properties System\Materials\1,2-DICHLOROETHANE

Property method template

PhastMC

General

Constants

Acentric factor	0.286595	
Aerosol class number		
Critical pressure	53.7	bar
Critical temperature	288.45	degC
Flammable/Toxic flag	Flammable	
Melting point	-35.66	degC
Molecular weight	98.9592	
Normal boiling point	83.444	degC
Reactivity with atmosphere	Not Strongly Reactive	
SRK alpha calculation flag		
Triple point pressure	0.00237127	bar
Triple point temperature	-35.66	degC

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	4.5507E+07	0.34444	0	0	0	-35.66	288.45	1	Constant value above fraction Tc

Flammable



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Page 1 of 7

Constants

Combustion at	0.895833	
Combustion ct	0.0775194	
Emissive power length scale	2.75	m
Flash point	12.85	degC
Heat of combustion	1.105E+06	kJ/kmol
Immediate ignition category	Unknown	
Laminar burning velocity		m/s
Lower flammability limit	62000	ppm
Luminous/Smoky flame flag	Smoky	
Maximum burn rate	0.04	kg/m2.s
Maximum surface emissive power	130	kW/m2
Pool fire burn rate length	0.1	m
TNT explosion efficiency		%
Upper flammability limit	160000	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

Toxic property B

Toxic property N

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	0.214	-0.000266	0	0	0	-20	83.44	1	Constant value above fraction Tc
Liquid viscosity	101	15.312	-41.12	-3.919	0	0	-35.66	126.85	1	Constant value above fraction Tc
Surface tension	106	0.080837	1.2445	0	0	0	-35.66	288.45	1	Constant value above fraction Tc
Vapour thermal conductivity	102	0.00021054	0.9574	1414	0		83.44	726.85	1	None (use equation)
Vapour viscosity	102	1.4321E-07	0.7785	98.159	0		-35.66	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
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Ideal gas heat capacity	107	65271	112540	1737.6	87800	795.45	-73.15	1226.85	1	None (use equation)
Liquid heat capacity	100	179170	-444.74	0.93009	0	0	-35.66	83.44	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	92.355	-6920.4	-10.651	9.1426E-06	2	-35.66	288.45	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	1.2591	0.27698	561.6	0.30492	-35.66	288.45	1	Constant value above fraction Tc

Virial

Coefficients

Name	Equation	A	B	C	D	E	Minimum temperature	Maximum temperature	Fraction of critical	Supercritical extrapolation
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							ature [degC]	ature [degC]	temper ature [fraction]	lation
Second virial equation coefficient	104	0.1539	-167.77	-2.6786 E+07	8.0024E +18	-4.9925 E+21	-30.15	1226.85	1	None (use equation)

Association

Constants

Acid association flag	Not Modelled
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Enthalpy interpolation range 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		
Liquid water enthalpy coefficient B		
Liquid water enthalpy coefficient C		
Liquid water enthalpy coefficient D		
Liquid water surface tension	0	N/m
Reaction with water model	None	
Solubility in water	0.85	
Water heat transfer coefficient	0	W/m2.degK

