

Stofdocument deel A

CAS-nr: 7790-94-5

Chloorsulfonzuur

ClHO₃S

VN-nr: 1754

GEVI: X88

Synoniemen: chloorzwavelzuur, monochloorzwavelzuur (Engels: chlorosulfonic acid)

Interventiewaarden		10 min.	30 min.	1 uur	2 uur	4 uur	8 uur
Voorlichtingsrichtwaarden	VRW (mg/m³)	0,12	0,12	0,12	0,12	0,12	0,12
Alarmeringsgrenswaarden	AGW (mg/m³)	15	11	9,0	7,5	6,2	5,1
Levensbedreigende waarden	LBW (mg/m³)	120	89	74	61	51	42
Datum vaststelling: 06-10-2016		1 mg/m ³ = 0,206 ppm; 1 ppm = 4.846 mg/m ³					
Explosiegrens: geen, maar stof reageert heftig tot explosief bij contact met water.			Geur: sterke stekende geur				
			LOA: niet afgeleid				
Fysisch-chemische eigenschappen				Overige informatie			
Uiterlijk: kleurloze tot lichtgele vloeistof		Molecuulmassa: 116,5 g/mol		Publieke grenswaarde: niet afgeleid			
Brand: bij vele reacties kans op brand en explosie		Zuurgraad: pH <1		MAK: niet afgeleid			
		LogKow: geen data		TLV-TWA: niet afgeleid			
Relatieve dichtheid van verzadigd damp-lucht mengsel: 1,0		Wateroplosbaarheid: reactie					
		Verzadigde dampdruk: 0,5 mbar					
Toxicologische eigenschappen							
Effecten bij inhalatoire blootstelling				Toxiciteit bij eenmalige, inhalatoire blootstelling			
<u>Onder VRW:</u> lichte irritatie aan de ogen				<ul style="list-style-type: none"> Blootstelling aan de stof kan ernstige chemische brandwonden veroorzaken. De damp van de stof werkt bijtend op de ogen, de huid en de luchtwegen. Inademing van de damp kan bronchitis en longoedeem veroorzaken, echter uitsluitend na verschijnselen van bijtende effecten op de slijmvliezen van ogen en/of hogere luchtwegen. De verschijnselen hiervan kunnen vertraagd optreden en versterkt worden door lichamelijke inspanning. In ernstige gevallen kans op verstikking door zwellingen in de keel en/of dodelijke afloop. De stof ontleed bij verhitting en vorm dan o.a. chloorwaterstof en zwaveldioxide. In contact met vocht vorming van o.a. zoutzuur en zwavelzuur; bij contact met warm water en waterdamp zeer heftig tot explosief; de stof vormt aan de lucht giftige en bijtende nevels 			
<u>VRW → AGW:</u> keelpijn en hoesten, rode en pijnlijke ogen, tranenvloed, branderig gevoel achter het borstbeen, moeizaam ademen							
<u>AGW → LBW:</u> brandwonden, troebel zicht, blindheid, kortademigheid, ademnood							
<u>Boven LBW:</u> ernstige kortademigheid, ademnood, kans op sterfte							
Effecten bij blootstelling aan vloeistof				Carcinogeniteit			
<u>Huidcontact:</u> bijtend, roodheid en pijn, blaren, ernstige brandwonden.				IARC classificatie: niet geclassificeerd*			
<u>Oogcontact:</u> bijtend, roodheid en pijn, ernstige brandwonden, verlies van gezichtsvermogen.				CRP: niet afgeleid			
				* de stof zelf is niet geclassificeerd, maar H ₂ SO ₄ bevattende mist wel (cat 1, IARC 2012).			
Beknopte medische informatie							
Ontsmetting damp							
<i>algemeen:</i> frisse lucht, rust, halfzittende houding, direct spoedeisende medische hulp inzetten							
Ontsmetting vloeistof							
<i>huid:</i> bij verbranding aan de huid vastgeplakte kleding NIET lostrekken, spoelen met veel water / kleding verwijderen, direct spoedeisende medische hulp inzetten.							
<i>ogen:</i> minimaal 15 min. spoelen met water (evt. contactlenzen verwijderen), dan naar oogarts brengen, blijven spoelen tijdens vervoer.							
<i>inslikken:</i> mond laten spoelen (uitspugen!), GEEN braken opwekken, direct spoedeisende medische hulp inzetten.							
Specifieke behandeling en materialen: geen.							
Neem contact op met het NVIC (Tel:+31 (0)30 274 8888) voor informatie met betrekking tot medisch handelen							

Stofdocument deel B

CAS-nr: 7790-94-5

Chlorosulfonic acid ClHO_3S

UN-nr: 1754

Basis for the Dutch Intervention Values

VRW: Based on sulfuric acid, in accordance with AEGL, 2 hr value added.

AGW: Same rationale as for AEGL (analogy with sulfuric acid values), but in contrast to AEGL-2 time-scaling is performed to derive values for other time points, 2h value added

LBW: Same point of departure as AEGL, but using different UF and different value for n, time-scaling applied to the 8 hour value, 2 hr value added.

Date: 06-10-2016

AEGL Document: Interim June 2008

Dutch Intervention Values (mg/m^3)

	10 min	30 min	1 h	2 h	4 h	8 h	End point
VRW	0.12	0.12	0.12	0.12	0.12	0.12	Based on sulfuric acid (nondisabling irritation in humans)
AGW	15	11	9.0	7.5	6.2	5.1	Based on sulfuric acid (absence of AGW effects in humans)
LBW	120	89	74	61	51	42	Threshold of rat lethality

Derivation of the Dutch Intervention Values

Chlorosulfonic acid is a strong corrosive acid and hydrolyzes exothermically *in situ* upon contact with moist mucous membranes to form equimolar amounts of the strong corrosive acids HCl and H_2SO_4 . Animal studies indicated that chlorosulfonic acid is more acutely toxic than HCl or H_2SO_4 , or a mixture of HCl + H_2SO_4 , but do not allow determination of the relative toxicities of these chemicals. Because no human or animal studies were available for derivation of the VRW and AGW, the values are based on the structural analogy to H_2SO_4 . This approach is considered valid because H_2SO_4 is a rapid hydrolysis product of, and is structurally related to, chlorosulfonic acid, and the two compounds have a similar mode of toxicity (eye and respiratory irritants).

VRW: Since no appropriate data exist for chlorosulfonic acid, VRW values for sulfuric acid will be used (on molar-basis) to derive VRW values for chlorosulfonic acid. The use of sulfuric acid as a surrogate for chlorosulfonic acid was deemed appropriate, because H_2SO_4 is a rapid hydrolysis product of, and is structurally related to, chlorosulfonic acid, and the two compounds have a similar mode of toxicity (eye and respiratory irritants).

Derivation of VRW values for sulfuric acid

The results of various studies clearly indicate that the first signs of respiratory irritation that can be characterized as notable discomfort occur at concentrations higher than 0.05 ppm in humans, including exercising asthmatics, justifying an intraspecies factor of 1. It was concluded that the concentration of 0.05 ppm can be used as the point of departure for VRW. In the absence of good time-concentration effect data and considering the type of effect, the value of 0.05 ppm was flat-lined across the 10- and 30-minute, and the 1-, 2-, 4-, and 8-hour exposure time points. This approach was considered appropriate because mild irritant effects generally do not vary greatly with time, and is in line with the derivation of VRW values for other respiratory irritants.

Based on molecular weight correction the PoD for chlorosulfonic acid is $0.238 \text{ mg}/\text{m}^3$.

For chlorosulfonic acid a modifying factor (MF) of 2 was applied because chlorosulfonic acid is believed to be approximately 2-fold more toxic than sulfuric acid. This is because one molecule of chlorosulfonic acid yields a molecule of sulfuric acid as well as a molecule of HCl and heat, and removes a molecule of water upon hydrolysis in tissues.

AGW: Since no appropriate data exist for chlorosulfonic acid, AGW values for sulfuric acid will be used (on molar-basis) to derive AGW values for chlorosulfonic acid. The use of sulfuric acid as a surrogate for chlorosulfonic acid was deemed appropriate, because H_2SO_4 is a rapid hydrolysis product of, and is structurally related to, chlorosulfonic acid, and the two compounds have a similar mode of toxicity (eye and respiratory irritants).

Derivation of AGW values for sulfuric acid

Occupational studies indicate that no irreversible or other serious health effects or an impaired ability to escape are to be expected from single exposures to concentrations of up to 9 ppm. The

concentration of 6 ppm (8-hour exposure) was used as the point of departure for AGW. Under these exposure conditions workers were perfectly able to complete their work shift. An intraspecies uncertainty factor of 3 is needed to account for sensitive subpopulations. This results in an 8-hour AGW value of 2 ppm. This AGW level is considered to be rather conservative because no irreversible or disabling effects were observed following acute exposure to sulfuric acid in any of the relevant human volunteer studies. Time scaling was performed, with $n=3.7$ derived from LBW calculations for sulfuric acid.

Based on molecular weight correction the PoD for chlorosulfonic acid is 30.88 mg/m^3 . A modifying factor (MF) of 2 was applied because chlorosulfonic acid is believed to be approximately 2-fold more toxic than sulfuric acid. This is because one molecule of chlorosulfonic acid yields a molecule of sulfuric acid as well as a molecule of HCl and heat, and removes a molecule of water upon hydrolysis in tissues.

LBW: The highest non-lethal concentration of 735 mg/m^3 in an 1-hour acute inhalation toxicity study with rats was used as point of departure for the derivation of the LBWs. Clinical effects were observed at 1 hour of exposure to $379\text{-}735 \text{ mg/m}^3$ and at $1539\text{-}3096 \text{ mg/m}^3$ all but one animal died. In contrast to the AEGL, the default total uncertainty factor of 10 (3×3) was considered sufficient to account for inter- and intraspecies differences. Time scaling was performed using $C^n \cdot t = k$, with the n -value of 3.7 for sulfuric acid. In absence of a substance-specific n -value for chlorosulfonic acid, taking into account that sulfuric acid is formed upon hydrolysis of chlorosulfonic acid, and the similar working mechanism of both substances, this was considered appropriate.

Additional toxicological information (including relevant results of a general literature search, if any)

Chlorosulfonic acid is a strong corrosive acid, and hydrolyzes exothermically *in situ* upon contact with moist mucous membranes to form equimolar amounts of the strong corrosive acids HCl and H_2SO_4 . It is unknown to what degree chlorosulfonic acid and/or its hydrolysis products contribute to chlorosulfonic acid toxicity, although each is capable of lowering tissue pH at the contact site and causing cellular destruction. Consistent with contact-site toxicity, the respiratory system was the initial target organ for chlorosulfonic acid, HCl, and H_2SO_4 in animal inhalation studies. However, since chlorosulfonic acid hydrolysis also produces heat and uses a molecule of water for each molecule of hydrolyzed chlorosulfonic acid, it is likely that there are some differences in the toxicity of chlorosulfonic acid, HCl, and H_2SO_4 . Animal studies indicated that chlorosulfonic acid is more acutely toxic than HCl or H_2SO_4 , or a mixture of HCl + H_2SO_4 .

No animal data were found on developmental and reproductive toxicity and genotoxicity upon inhalation exposure. The chlorosulfonic acid hydrolysis products HCl and H_2SO_4 do not appear to have significant developmental or reproductive toxicity, but both have some genotoxic potential. No carcinogenicity data for chlorosulfonic acid were available. But based on occupational data, IARC concluded that strong-inorganic acid mists containing sulfuric acid are carcinogenic to humans.

H314: Causes severe burns and eye damage, H335: May cause respiratory irritation

It is noted that the observed considerable variation among studies in the exposure concentration causing lethality is likely due to difficulty in achieving and maintaining the target chlorosulfonic aerosol concentrations.

Carcinogenicity and derivation of the CRP value

IARC classification: not classified
(Strong-inorganic-acid mists (containing H_2SO_4) are carcinogenic to humans (group 1))
No carcinogenic risk potency (CRP) was derived, because not suitable data are available.

Odour and derivation of the LOA value

Odour: strong and pungent odour
No LOA was derived, because no information was found regarding the threshold of awareness and recognition.

Other standards and guidelines (1h values in mg/m^3 , unless otherwise indicated)

VRW level 0.12	AEGL-1 0.10	ERPG-1 2	IDLH: -
AGW level 9.0	AEGL-2 4.4	ERPG-2 10	
LBW level 74	AEGL-3 25	ERPG-3 30	