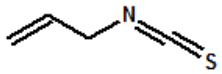
Allyl isothiocyanate

CAS-No.:	57-06-7 The scope of this Standard includes, but is not limited to the CAS number(s) indicated above; any other CAS number(s) used to identify this fragrance ingredient should be considered in scope as well.	**Molecular formula:**	$C_4H_5N_5$
		Structure:	
Synonyms:	Allyl isosulfocyanate Allyl thiocarbonimide 1-Propenal, 3-isothiocyanato- 2-Propenyl isothiocyanate AITC		

History:	Publication date:	2020 (Amendment 49)	Previous Publications:	2008

Implementation dates:	For new submissions*:	February 10, 2021
	For existing fragrance compounds*:	February 10, 2022
	*These dates apply to the supply of fragrance mixtures (formulas) only, not to the finished consumer products in the marketplace.	

RECOMMENDATION:	**PROHIBITION**

FRAGRANCE INGREDIENT PROHIBITION:	Allyl isothiocyanate as such should not be used as a fragrance ingredient. The natural extracts containing Allyl isothiocyanate should not be used as substitutes for this substance.

CONTRIBUTIONS FROM OTHER SOURCES:	**SEE ANNEX I**

Allyl isothiocyanate

ANNEX I Natural Complex Substances (NCS) containing Allyl isothiocyanate					
Concentration in NCS (%)	CAS number of ingredient	Name of NCS	Botanical name	CAS number of NCS	Essential oil category
61.5	57-06-7	Mustard oil	Brassica spp.	8007-40-7	H2.12
45	57-06-7	Horseradish oil	Amoracia rusticana G. Gaertn. et al.	84775-62-2	A2.12

Allyl isothiocyanate can be found at relatively high levels in Mustard oil and Horseradish oil. The natural extracts containing Allyl isothiocyanate should not be used as substitutes for this substance. This means that the use of Mustard oil and Horseradish oil cannot be considered safe and therefore both extracts should not be used in fragrance mixtures until additional data is available and considered sufficient to support the safe use of these ingredients.

This is a non-exhaustive indicative list of typical natural presence for Allyl isothiocyanate and is intended to be used in the absence of own analytical data. If analysis has shown that the level of the restricted ingredient in a natural complex substance is different from what is provided in this Annex I, then the analytically determined level should be used in place of the indicative level.

It should further be noted that natural complex substances themselves can be restricted by an IFRA Standard.

For a detailed list of natural contributions, please refer to the Annex I of IFRA Standards, publicly available on the IFRA website (www.ifrafragrance.org).

INTRINSIC PROPERTY DRIVING RISK MANAGEMENT:	**INSUFFICIENT DATA**

EXPERT PANEL FOR FRAGRANCE SAFETY RATIONALE / CONCLUSION:

The Expert Panel for Fragrance Safety reviewed all the available data for Allyl isothiocyanate and recommends not to use Allyl isothiocyanate as or in fragrance ingredients in any finished product application until additional data is available and considered sufficient to support its safe use.

REFERENCES:

The IFRA Standard on Allyl isothiocyanate is based on at least one of the following publications:

• The RIFM Safety Assessment on Allyl isothiocyanate if available at the RIFM Safety Assessment Sheet Database: http://fragrancematerialsafetyresource.elsevier.com

• Api A.M., Belsito D., Bruze M., Cadby P., Calow P., Dagli M. L., Dekant W., Dent M., Ellis G., Fryer A. D., Fukayama M., Griem P., Hickey C., Kromidas L., Lalko J., Liebler D.C., Miyachi Y., Politano V.T., Renskers K., Ritacco G., Salvito D., Schultz T.W., Sipes I. G., Smith B., Vitale D., Wilcox D.K. (2015). Criteria for the Research Institute for Fragrance Materials, Inc. (RIFM) safety evaluation process for fragrance ingredients. Food Chem Toxicol. 2015 Aug;82 Suppl:S1-S19 (http://fragrancematerialsafetyresource.elsevier.com/sites/default/files/Criteria_Document_Final.pdf).

• IDEA project (International Dialogue for the Evaluation of Allergens) Final Report on the QRA2:

Allyl isothiocyanate

Skin Sensitisation Quantitative Risk Assessment for Fragrance Ingredients, September 30, 2016 (http://www.ideaproject.info/uploads/Modules/Documents/qra2-dossier-final--september-2016.pdf).

• Salvito D.T., Senna R. J., Federle T.W. (2002). A framework for prioritizing fragrance materials for aquatic risk assessment. Environ Toxicol Chem. 2002;21:1301-1308 (https://www.ncbi.nlm.nih.gov/pubmed/12069318).

Additional information on the application of IFRA Standards is available in the Guidance for the use of IFRA Standards, publicly available at www.ifrafragrance.org.