ID Card
Aurio(1+) 2,6,6-trimethylbicyclo[3.1.1]heptanethiolate

Version 4 July 2023

Notes:

- *This ID card is used to support the substance sameness discussions in SIEFs and to describe the substance to the best of the SIEF members' knowledge.*
- *It also aims at grouping communications relevant to the request of available data or information, the approval of the proposed Lead Registrant and the registration strategy with the SIEF.*
- *It is the responsibility of each individual registrant to identify their substance and to report company-specific identity in their Registration Dossier (section 1 of IUCLID).*
- *All blue text is intended as guidance and can be removed from the final ID card. Text in <> should be replaced as appropriate.*
- *For numerical entries, a comma is used as decimal mark and a point is used as thousands separator.*
- *Several compositions, forms and techniques can be provided for one substance, by completing one ID Card/relevant table for each one.*

1. Identification of the substance

Table 1. Identification of the substance

	Original (in EC inventory)
Name	Aurio(1+) 2,6,6-trimethylbicyclo[3.1.1]heptanethiolate
EC number	269-858-3
CAS number	68365-87-7
Description	Not available
Composition type	Mono-constituent substance

2. Synonyms and other identifiers of the substance

Add / remove rows / identifiers as necessary. If no synonyms / other identifiers are available, replace below table by 'None'.

Table 2. Synonyms and other identifiers of the substance

IUPAC name	aurio(1+) 2,6,6-trimethylbicyclo[3.1.1]heptanethiolate
CAS name	aurio(1+) 2,6,6-trimethylbicyclo[3.1.1]heptanethiolate
Abbreviations	
Other commercial, brand or international names	Gold pinanyl mercaptide Gold mercaptide Bicyclo[3.1.1]heptanethiol, 2,6,6-trimethyl-, gold(1+) salt
Other identity codes	EINECS 269-858-3

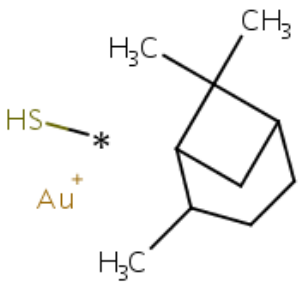
3. Substances (with core identifiers) also falling under this substance (with justification)

None

4. Information related to molecular and structural formula of the substance

If any of below information is not available / not applicable, please indicate so.

Table 3. Information related to molecular and structural formula of the substance

Molecular formula	C10H18S.Au
Structural formula	
Smiles notation	[Au+].C1[C@@H]([C@@H]2C([C@@H](C1)C2)(C)C)C.*S
Optical activity	Not applicable
Typical ratio of (stereo) isomers	Not applicable
Molecular Weight / Molecular Weight range	368.296 g/mol

5. Typical composition of the substance

Please indicate in the below table clear boundaries of the constituents that characterise the substance. The composition of the substance should be reported in line with what is analytically measured.

Impurities present in concentrations < 1% should only be reported if they potentially influence the classification.

Table 4. Typical composition

	Name	Symbol / Formula	Min & Max concentrations (%)	Typical concentration (range) (%)
Main constituent(s)*	Aurio(1+) 2,6,6-trimethylbicyclo[3.1.1]heptanethiolate	C10H18S.Au	94 – 96,5	96
Additive(s)**				
Main impurity(-ies)#	2,6,6-trimethylbicyclo[3.1.1]heptane-3-thiol disulphide	C10H18S3	2 - 3	2
	2,6,6-trimethylbicyclo[3.1.1]heptane-2-thiol disulphide	C10H18S3	1 - 2	1.5
Other impurities##	2,6,6-trimethylbicyclo[3.1.1]heptane-1-thiol	C10H18S	0.5 - 1	0.5

* ≥ 80 % (w/w) for mono-constituent substances; ≥ 10 % (w/w) and < 80 % (w/w) for multi-constituent substances.

** ≥ 1 % (or lower if contributing to the hazard). An additive is a substance that has been intentionally added to stabilise the substance and which cannot be removed without changing the chemical nature to which it is added.

≥ 1 %. An impurity is an unintended constituent present in a substance, as produced. It may originate from the starting materials or be the result of secondary or incomplete reactions during the production process. While impurities are present in the final substance, they were not intentionally added.

< 1 % and potentially influencing the classification of the substance.

The composition given above is typical and should therefore represent the majority of Aurio(1+) 2,6,6-trimethylbicyclo[3.1.1]heptanethiolate as manufactured and/or imported in the EEA market. Aurio(1+) 2,6,6-trimethylbicyclo[3.1.1]heptanethiolate containing less than <typical concentration> <main constituent> may still be considered to be the same for the purpose of registration under REACH and may be referred to as impure Aurio(1+) 2,6,6-trimethylbicyclo[3.1.1]heptanethiolate to distinguish if from the typically pure Aurio(1+) 2,6,6-trimethylbicyclo[3.1.1]heptanethiolate.

6. Information on appearance, physical state and properties of the substance

Use Table 5 for solids and **Error! Reference source not found.** *for solutions. Delete as appropriate.*

The Lead Registrant should provide a picture of the substance in its various forms to be added to the ID card.

Table 5. Appearance / physical state / properties of the solid substance

Physical state	Solid
Physical form*	Amorphous
Appearance	Pale yellow powder
Particle size**	Coarse powder
Does the substance contain 'bound water'?#	No
Does the substance contain 'crystallisation water'?#	No
Does the solid hydrolyse?##	No
Is the solid hygroscopic?§	No

* Crystalline form: solid material whose constituent atoms, molecules, or ions are arranged in an ordered pattern extending in all three spatial dimensions. Amorphous form: solid material whose constituent atoms, molecules, or ions are randomly arranged.

** Nanoform: particles in the size range 1 - 100 nm (for definition of a nanomaterial, see http://ec.europa.eu/environment/chemicals/nanotech/faq/definition_en.htm). Fine powder: particles in the size range 100 – 2.500 nm. Coarse powder: particles in the size range 2.500 nm – 1 mm. Massive object: particles in the size range > 1 mm.

'Bound water': water molecules that are coordinated as bound ligands. 'Crystallisation water' or hydration water: water that occurs in crystals (necessary for the maintenance of crystalline properties) but which is not directly bound to the metal ion (a hydrate contains a definite % of crystallisation water e.g. $CuSO_4 \times 5 H_2O$, an anhydride does not contain any water)

Hydrolysis: decomposition (cleavage of chemical bonds) by the addition of water.

§ Hygroscopic substance: readily attracts moisture from its surroundings in open air, through either absorption or adsorption.

7. Analytical data

Annex VI of REACH requires the registrant to describe the analytical methods and/or to provide the bibliographical references for the methods used for identification of the substance and, where appropriate, for the identification of impurities and additives. This information should be sufficient to allow the methods to be reproduced.

The table below lists analysis methods applicable to precious metal and / or rhenium substances. The Lead Registrant should indicate which methods they usually apply for identification of the substance by ticking the appropriate boxes in below table. EPMF should then complete with acceptable alternatives and / or additional requirements.

Comments on the applicability of the techniques are welcome, but should be added in a text paragraph under the table.

Table 6. Analytical methods for identification of the substance

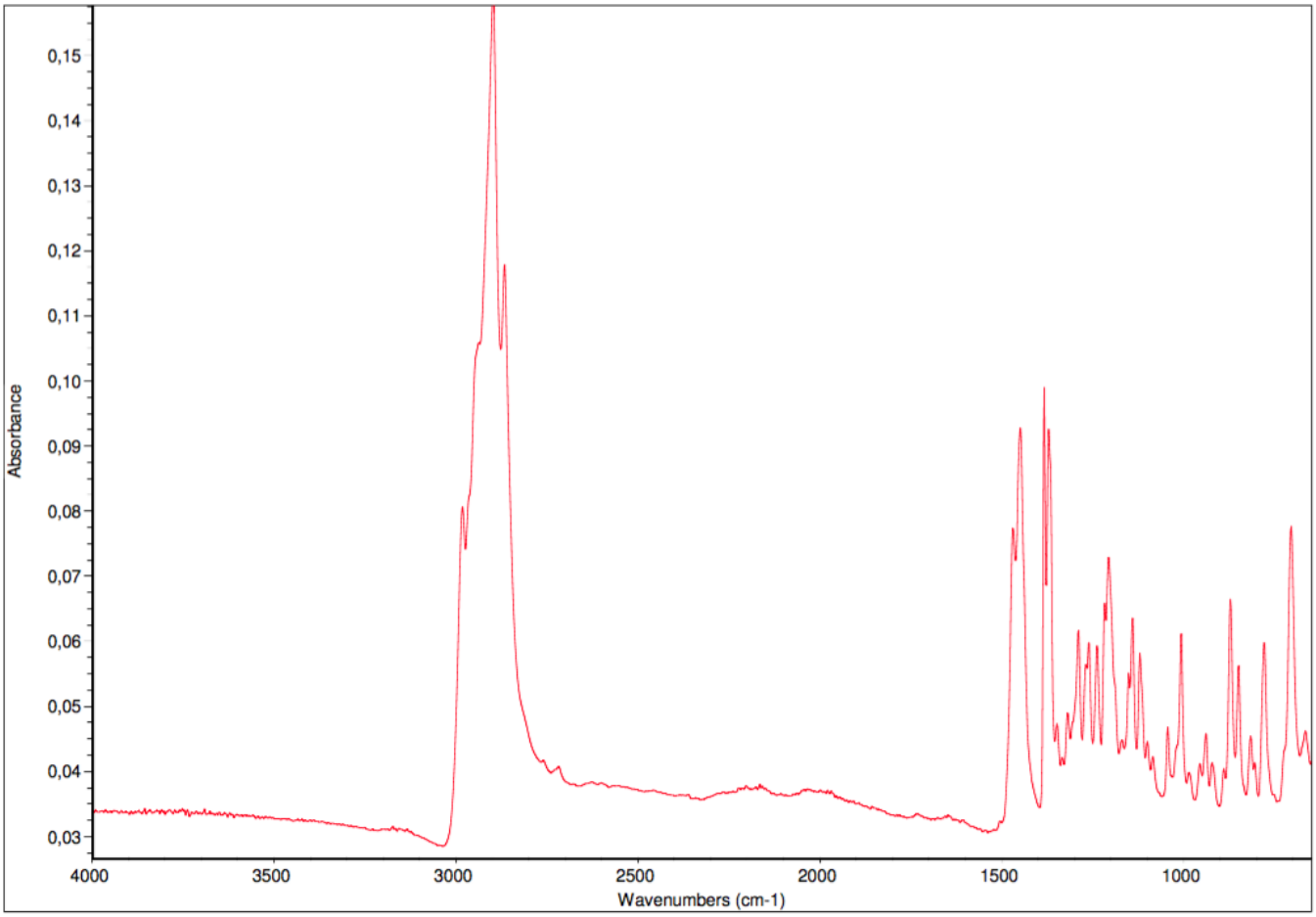
Parameter / Method	Recommended for substance identification and sameness check	Applicable	Not applicable or not recommended
Elemental analysis			
ICP (ICP-MS or ICP-OES)	X		
Atomic absorption spectroscopy (AAS)			
Glow discharge mass spectrometry (GDMS)			
Molecular analysis			
Infrared (IR) spectroscopy	X	X	
Raman spectroscopy		X	
Mineralogical analysis			
X-Ray Fluorescence (XRF)		X	
X-Ray Diffraction (XRD)	X	X	
Morphology and particle sizing			
Electron microscopy (SEM, TEM, REM)* #			
Laser diffraction* #	X		
Particle size by other means (e.g. sieve analysis)#			
Surface area by N-BET* #	X	X	
Other			

* Analytical techniques particularly (but not exclusively) relevant for nanomaterials.

The choice of the technique for particle size depends on the size of the material as manufactured/imported/placed on the market/used.

Aurio(1+) 2,6,6-trimethylbicyclo[3.1.1]heptanethiolate - Analytical Reference Information

Fourier transformed IR spectra of Aurio(1+) 2,6,6-trimethylbicyclo[3.1.1]heptanethiolate



8. Lead Registrant

Fenzi AGT Netherlands B.V. (The Netherland) volunteers to be the Lead Registrant for Aurio(1+) 2,6,6-trimethylbicyclo[3.1.1]heptanethiolate. The EPMF will provide support to the Lead Registrant as laid down in the EPMF Agreement.

9. Scope of the Registration Dossier

The uses included in this Registration Dossier are listed on the EPMF website.