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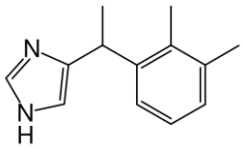
Technical data sheet
Selektope

Product description

Selektope is an effective antifouling agent patented and developed by I-Tech AB. It can be used in antifouling coatings for ship and boat hulls and in coatings for other submerged marine structures.

Identity

CAS-No. **EINECS-no**	86347-14-0 Not listed
IUPAC Name	4-[1-(2,3-dimethylphenyl)ethyl]-*1H*-imidazole
Other common name	Medetomidine
Molecular formula	$C_{13}H_{16}N_2$
Structural formula	
Molecular weight (g/mol)	200,28 g/mol

Specifications

Purity (HPLC)	≥96.5%
Assay (HPLC)	96.5-103.4%
Any unknown impurity	≤0.54%
Loss on drying	≤1.44%
Water content	≤ 0.54%
Enantiomeric composition	Racemic

Physical and chemical properties

Colour	White or Almost white or Off white or Slightly yellow or Light yellow or Yellow or Light brown
Physical state	Crystalline powder
Odour	Odourless
Melting point	110-116°C
Boiling point	386°C (DSC, 1013 mbar) but decomposition starts at about 150°C resulting in a brownish melt.
Relative density	1.113g/cm^3
Vapour pressure	3.5 x 10^{-6} Pa at 20°C, 8.3 x 10^{-6} Pa at 25°C
Dissociation constant	pK_b = 6.9
Partition coefficient	Log P_{ow} = 3.1

Solubility and stability

Solubility of Selektope in water and buffer systems

pH	Temperature (˚C)	Solubility (g/l)
5	10	9.75
	20	9.86
	30	12.1
7	10	0.353
	20	0.425
	30	0.489
9	10	0.0834
	20	0.153
	30	0.189

The methods followed are amongst those described in Commission Regulation (EC) No. 440/2008 (Method A.6) and the OECD Guidelines for the Testing of Chemicals (Method 105).

Solubility and stability of Selektope in organic solvents

Solvent	Solubility of Selektope [g/L]					Stable / Degradation [%] #
	0°C	10°C	20°C	30°C	40°C	14 days at 54 °C
1-methoxy-2-propanol [A]	≥250	≥250	≥250	≥250	≥250	Stable
benzyl alcohol [B]	≥250	≥250	≥250	≥250	≥250	Stable
p-xylene	*	1.6	2.6	6.2	26	Stable
o-xylene	0.92	1.9	3.8	11	66	Stable
acetone [C]	21	32	48	120	170	Stable
ethyl acetate	11	17	25	53	86	Stable
methanol	≥250	≥250	≥250	≥250	≥250	Stable
acetonitrile	6.2	12	17	29	53	Stable
methylisobutyl ketone[D]	20	27	36	56	80	Stable / 8
2-methoxy-1-methylethyl acetate	12	17	24	44	63	Stable
iso-butanol	≥250	≥250	≥250	≥250	≥250	Stable
n-butanol[E]	≥250	≥250	≥250	≥250	≥250	Stable

Selektope was considered being stable if there was less than 5% degradation after 14 days at 54°C. In most tested solvents, there was -2% to 2% degradation which is considered to be within the measuring error.
*Measurement was not possible due to that the sample was frozen under those conditions.
[A] In another experiment, it was determined that the solubility of Selektope was 341 g/L at 25°C.
[B] In another experiment, it was determined that the solubility of Selektope was >650 g/L at 25°C.
[C] Reaction with acetone has been noted at elevated temperatures and high pH. There was however, no reaction with acetone observed during this stability test.
[D] In methylisobutyl ketone, 8% disappeared over the observation time caused by a reaction with an impurity (mesityl oxide) which is commonly present in this solvent.
[E] In another experiment, it was determined that the solubility of Selektope was ~460 g/L at 25°C.

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Shelf life

The shelf life of Selektope is 4 years from production date taken that it is properly stored in a closed container under dry and dark conditions. Each commercial delivery is accompanied with a certificate of analysis (CoA). The CoA states a retest date that is four years after the production batch's original release date or its latest retest date. Material that has passed the retest date is in most cases unaltered; however, a retest should be performed to ensure quality.

Biological properties:

Effective concentrations

Selektope will hinder barnacle larvae from settling in as low concentration as 5pg/l in sea water. In practice, an addition of 0.2 % of Selektope calculated on weight per dry weight paint is often enough for protection against barnacles.

Mode of action

Selektope specifically targets the octopamine receptor in the barnacle larva. This receptor triggers a behaviour causing the larva to swim away. Selektope is hence a deterring substance. The effect is temporal and reversible and the larva will regain its normal behaviour once it has left the treated surface.

Target species and non-target species

Selektope's main target are barnacles but is also to some extent effective against other hard fouling organisms such as tube worms. Selektope does not have any effect on non-target species at the predicted environmental concentration (PEC). Selektope does not bio-accumulate in fish, shellfish or any other marine organisms tested.

Workers health

Proper personal protective equipment (PPE) should **always** be worn when handling Selektope. PPE should include safety goggles, protective gloves, dust mask and protective clothing. For further instructions, please see the material safety data sheet and the safe use guideline. Both are available upon request from I-Tech.

How to use Selektope in antifouling paint

To obtain a full protection against fouling organisms, 0.1 - 0.3% dry weight of Selektope should be used in paints together with one or more algaecide.

Interaction between Selektope and other paint components

Selektope may interact with some common paint ingredients. Ionic and acid base interaction is possible with polymers and rosin containing acidic groups such as carboxylic acids. Selektope will also coordinate to metal ions and metal oxide such as zinc oxide and cuprous oxide. This has been shown to be an effective way to control the release of Selektope and prevent premature depletion of the paint film. It is believed that Selektope is released at the same rate as the carrier is dissolved or hydrolyzed.

Technical benefits

- Selektope is not corrosive in any way and hence, can be used on all kinds of substrates including aluminium.
- Selektope is colourless in itself therefore paint formulations with bright colours are possible.

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