

Substance Identity Card for TOS	
Substance name	Tall Oil Soap
Reference substance name ¹	Alkaline Aqueous Extraction of sodium salts of fatty acids and rosin acids from the Kraft Pulping Process
EINECS	266-037-1
REACH Substance description ²	<p>Tall Oil Soap (TOS) is generated in the Kraft Pulping Process and is separated from spent liquors as a by-product. It is a dark brown sticky viscous liquid or paste extracted from softwoods and hardwoods.</p> <p>TOS has a complex composition of sodium salts of fatty acids and rosin acids, sterols, lignin and cellulose fibre. Its composition varies. The main blocks are:</p> <ul style="list-style-type: none"> • 5-45% w/w sodium salts of saturated and unsaturated C14-C20 fatty acids • 10-40% w/w rosin acid sodium salts • 25-45% w/w water • 1-10% w/w sterols • 3-20% w/w lignin, cellulose fibre and oligomeric acids
CAS Name	Tall Oil, sodium salt
CAS number	65997-01-5
Synonyms	<p>Tall Oil Soap, TOS Crude Tall Oil Soap Black liquor soap Tall Oil, sodium salt (EINECS name)</p>
Type of substance ³	UVCB
General information of the manufacture process for the boundary composition	<p>- Identity of starting materials/source (and ratio): The source material is spent liquor from wood pulping.</p> <p>- Reaction steps/mechanisms: Tall oil soap is generated by the pulp and paper industry during the Kraft Pulping Process. The fatty and rosin acids in the tree species used to produce wood pulp are saponified during the alkaline cooking due to the alkaline conditions in the digester and forms sodium soaps which dissolve in the black liquor (spent liquor). In the cooking process, lignin and carbohydrates are dissolved and the fibres are liberated by treating wood chips with cooking liquor at high temperature approximately 170°C and at elevated pressure, approximately 790 kPa. The black liquor is the aqueous solution of dissolved organic material and spent cooking chemicals.</p> <p>- Relevant operating parameters (e.g. temperature and pressure): Temperature of approximately 170°C and elevated pressure of approximately 790 kPa.</p> <p>- Solvents/reagents used: Kraft pulping reagents</p> <p>- Details on any extraction/isolation steps as appropriate: In the chemical recovery process the soap separates from the water phase and forms a soap layer on the liquor surface as the black liquor is successively concentrated and the solubility of the soap is decreased.</p>

Foot note	Section in the IUCLID6
1	Section 1.1 Reference substance name Section 1.1 Reference substance information/IUPAC name field
2	Section 1.1 Reference substance information /Description
3	Section 1.1 Type of substance

	<p>- Details on any clean-up/purification steps as appropriate: For process reasons most of the soap has to be removed from the black liquor in order to avoid foaming in the evaporators and to maintain stable combustion in the recovery boiler.</p> <p>- Physical-chemical parameters (e.g. boiling point): The separation of Tall Oil Soap depends on the solubility of the soap and the rising velocity of the soap droplets. The soap solubility decreases as the dry substance content of the black liquor is increased and reaches a minimum at about 25 % DS.</p>
Typical composition of major constituents	<ul style="list-style-type: none"> • 32% w/w water (CAS 7732-18-5, EC 231-791-2) • 7% w/w sodium oleate (CAS 143-19-1, EC 205-591-0) • 9% w/w sodium linoleate (CAS 822-17-3, EC 212-491-0) • 10% w/w sodium abietate (CAS 14351-66-7, EC 238-313-1) • 4% w/w sodium dehydroabietate (CAS 37206-28-3, EC 248-873-9) • 10% w/w lignin, cellulose fibres and oligomeric acids
Note	Tall oil soap has been given two different classifications depending on its pH value; 9-11.5 or >11.5

Boundary composition ranges of TOS					
	Constituents grouped into blocks	CAS No	EC No	Concentration (% w/w)	
				Min	Max
BLOCK 1	Sodium salts of saturated and unsaturated C14-C20 fatty acids	None	None	5	45
BLOCK 2	Rosin acid sodium salts	None	None	10	40
BLOCK 3	Water	7732-18-5	231-791-2	25	45
BLOCK 4	Terpenes	None	None	0.0	0.1
BLOCK 5	Sesquiterpenes	None	None	0	1
BLOCK 6	Abietenes and labdanes	None	None	0	2
BLOCK 7	C30 branched polyalkanes	None	None	0	1
BLOCK 8	3,5-Dimethoxystilbene	None	None	0	0.5
BLOCK 9	Rosin alcohol and aldehydes isomers	None	None	0	3
BLOCK 10	C20-C35 alcohols and terpene alcohols	None	None	0	2
BLOCK 11	Sterols	None	None	1	10
BLOCK 12	Lignin, cellulose and fibre	None	None	3	20
	pH			pH >9	

Named constituents that could be present at greater than 10% and useful for sameness analysis

	Constituents grouped into blocks	CAS No	EC No	Concentration (% w/w)	
				Min	Max
	Sodium oleate	143-19-1	205-591-0	1	10
	Sodium linoleate	822-17-3	212-491-0	5	20
	Sodium abietate	14351-66-7	238-313-1	2	25
	Sodium dehydroabietate	37206-28-3	248-873-9	1	15

Mapping of current Blocks with the previous sameness Blocks						
Previous sameness names	Concentration (% w/w)			New Boundary Composition where constituents grouped into blocks	Concentration (% w/w)	
	Min	Max			Min	Max
Sodium salts of fatty acids	5	45	BLOCK 1	Sodium salts of saturated and unsaturated C14-C20 fatty acids	5	45
Sodium salts of resin acids	1	45	BLOCK 2	Rosin acid sodium salts	10	40
Volatiles (water and turpentine)	20	50	BLOCK 3	Water	25	45
			BLOCK 4	Terpenes	0.0	0.1
Neutrals (except other organics, volatiles and sodium)	0	20	BLOCK 5	Sesquiterpenes	0	1
			BLOCK 6	Abietenes and labdanes	0	2
			BLOCK 7	C30 branched polyalkanes	0	1
			BLOCK 8	3,5-Dimethoxystilbene	0	0.5
			BLOCK 9	Rosin Alcohol and aldehydes isomers	0	3
			BLOCK 10	C20-C35 alcohols and terpene alcohols.	0	2
			BLOCK 11	Sterols	1	10
			BLOCK 12	Lignin, cellulose and fibre	3	20