

TNHA

Tri-n-hexylaluminum

CAS Number	1116-73-0
EINECS/EC	2142416
Molecular Formula	(n-C ₆ H ₁₃) ₃ Al

APPLICATION

Tri-n-hexylaluminum (TNHA) can be used as a component of Ziegler-Natta catalysts for olefin and diene polymerizations. It may also be used to alkylate other metals or as an alkylating agent in organic syntheses. Certain transition metal salts may be reduced by tri-n-hexylaluminum.

SPECIFICATIONS

Aluminum, wt. %, min	9.0
TNHA, wt. %, min	95.0
Branched (C ₁₂ H ₂₅) ₃ Al, wt. %, max	2.0
Hydride (calculated as AlH ₃), wt. %, max	0.6
Hexene, wt. %, max	2.5

	Average (\bar{x})	Variation (3 σ)
Aluminum, wt. %	9.62	0.1
TNHA, wt. %	97.7	0.5
Branched (C ₁₂ H ₂₅) ₃ Al, wt. %	0.95	0.2
Hydride (calculated as AlH ₃), wt. %	0.25	0.12
Hexene, wt. %	< 0.15	(*)

(*) Insufficient data to determine sigma.

DENSITY AND VISCOSITY

Temperature		Density		Viscosity
°C	°F	g/mL	lbs/gal	cp
0	32	0.8541	7.127	69.7
10	50	0.8474	7.071	45.1
20	68	0.8407	7.015	30
25	77	0.8374	6.988	24.7
30	95	0.8341	6.96	20.4
40	104	0.8274	6.904	14.4
50	122	0.8207	6.848	10.2
60	140	0.814	6.792	7.4
70	158	0.8073	6.737	5.5
80	176	0.8007	6.681	4.1
90	194	0.794	6.625	3.1
100	212	0.7873	6.57	2.4
120	248	0.7739	6.458	1.5
140	284	0.7606	6.346	0.97
160	320	0.7472	6.235	0.66
180	356	0.7339	6.124	0.46
200	392	0.7205	6.012	0.33

Equations:

Density: $d(\text{g/rnL}) = 0.8541 - 0.000668t$; $t = \text{°C}$

Viscosity: $\log_{10}(\text{cp}) = -3.8963 + 1683.1/(t+293.25)$; $t = \text{°C}$

PHYSICAL PROPERTIES

Property	Value
Formula	(n-C ₆ H ₁₃) ₃ Al
Formula weight	282.49
State and color at 25°C	clear, straw-colored liquid
Stability in contact with air	fumes vigorously, may ignite spontaneously
Stability in contact with water	reacts violently
Density at 25°C (77°F), g/mL	0.8374
Melting point, °C(°F)	< -60 (-76)
Boiling point at 760 mm Hg (extrapolated), °C(°F)	308.5 (587.3)
Vapor pressure ¹ , mm Hg at:	
25°C (77°F)	0.0000047
40°C (104°F)	0.0000480
80°C (176°F)	0.007
120°C (248°F)	0.282
160°C (320°F)	4.39
220°C (428°F)	67.50
280°C (536°F)	396.00
Specific heat at 20°C, cal/g°C	0.5211
Specific heat at 68°F, btu/lb°F	0.5211
Heat of vaporization at NBP, cal/g	45.9
Heat of vaporization at NBP, btu/lb	82.7
ΔH° of formation at 25°C (77°F), kcal/gfw	-116.7
Heat of combustion at 25°C, cal/g	10,278
Heat of combustion at 77°F, btu/lb	18,502
Coefficient of volume expansion at 25°C, per °C	0.000804
77°F, per °F	0.000452
Heat of reaction with water at 25°C, cal/g	446
77°F, btu/lb	803

¹Decomposes below boiling point

SAFETY AND HANDLING

The pyrophoric nature of TNHA presents potential hazards not common to most liquid chemicals used by industry in tank truck quantities. TNHA, being pyrophoric, breaks into flame spontaneously and gives off dense smoke when exposed to air. It reacts violently with water. TNHA is a clear, noncorrosive mobile liquid with a low vapor pressure. Hydrocarbon solutions of TNHA, depending on the concentration and temperature, may not be pyrophoric. However, these solutions still must be blanketed with an inert gas such as dry nitrogen because TNHA will react with air and moisture at the surface of the solution, giving off dense smoke, heat and flammable gas. For specific information on the safe handling and toxicity of this product, please refer to the Material Safety Data Sheet, which is available upon request.

TRANSPORT & PACKAGING

Container Description	Nominal Value		Approximate Loadings	
	Gallons	Liters	Pounds	Kilograms
Tank Car (DOT-105A300W)	23,000-25,100	87,100-95,000	135,000-230,000	61,400- 104,000
Tank Trailer (DOT-MC330 or 331)	6,200-7,200	23,500-27,200	30,00-48,000	13,600- 21,800
Portable Tanks (DOT-51)/UN T21	430	1,635	2,250-3,800	1,021-1,725
	1,980	7,500	10,257-17,000	4,880-7,711
Isotank	5,635-5,970	21,330-22,600	30,000-34,000	13,600- 15,500
Cylinders: dual valve (DOT-4BA240)				
5 gallon size	5.7	22	25-53	11-24
26 gallon size	28.0	106	150-268	68-120
Laboratory cylinders (DOT-3AA2015)				
0.4 gallon size	0.40	1.47	1.2-2.2	0.58-0.97
1.0 gallon size	0.94	3.60	2.9-6.3	1.4-2.8

*Actual weight depends on highway load limits, product density and lifting considerations.

Shipments are made in accordance with DOT regulations — Section 173.134. All containers are shipped blanketed with dry nitrogen under slight positive pressure. Hydrocarbon solutions are also available blended to customer specifications. Tank rail cars and tank trucks are available in North America only.

Transportation Classification

Proper shipping name..... Organometallic Substance, Liquid, Pyrophoric, Water Reactive (Tri-n-hexylaluminum)
 Hazard class.....4.2 (spontaneously combustible) + 4.3(dangerous when wet)
 ID number..... UN3394
 Placard(s) spontaneously combustible w/ number 4+dangerous when wet 4
 Label(s)..... spontaneously combustible+dangerous when wet
 MARPOL Classificationn/a
 Harmonized tariff number2931.00.4000-2
 Schedule B number2931.00.6000-7

OTHER INFORMATION

Further Related Documents

Safety Data Sheet

The information presented herein is believed to be accurate and reliable, but is presented without guarantee or responsibility on the part of Albemarle Corporation and its subsidiaries and affiliates. It is the responsibility of the user to comply with all applicable laws and regulations and to provide for a safe workplace. The user should consider any health or safety hazards or information contained herein only as a guide, and should take those precautions which are necessary or prudent to instruct employees and to develop work practice procedures in order to promote a safe work environment. Further, nothing contained herein shall be taken as an inducement or recommendation to manufacture or use any of the herein materials or processes in violation of existing or future patent.

Technical data sheets may change frequently. You can download the latest version from our website www.albemarle.com.

Please contact us at www.albemarle.com/contact with questions.