

TNBA

Tri-n-butylaluminum

CAS Number	1116-70-7
EINECS/EC	214-240-0
Molecular Formula	(n-C ₆ H ₉) ₃ Al

APPLICATION

Tri-n-butylaluminum (TNBA) is used primarily as a catalyst component in Ziegler-Natta type systems for olefin and diene polymerizations. Other applications include use in alkylation reactions and as a catalyst component in linear oligomerization and cyclization of unsaturated hydrocarbons.

SPECIFICATION

Aluminum, wt. %	13.2
TNBA, wt. %	97.0
Branched (C ₆ H ₁₇) ₃ Al, wt. %	1.0
Hydride (calculated as AlH ₃), wt. %	0.1
Hydrocarbons, wt. %	1.8

	Average (\bar{x})	Variation (3 σ)
Aluminum, wt. %	13.5	0.1
TNBA, wt. %	99.4	0.1
Branched (C ₈ H ₁₇) ₃ Al, wt. %	0.4	0.2
Hydride (calculated as AlH ₃), wt. %	0.05	0.03
Hydrocarbons, wt. %	0.3	0.4

DENSITY & VISCOSITY

Temperature		Density		Viscosity
°C	°F	g/mL	lbs/gal	cp
0	32	0.841	7.018	28.4
10	50	0.834	6.959	19.6
20	68	0.827	6.901	13.6
25	77	0.8235	6.872	11.4
30	86	0.82	6.842	9.66
40	104	0.813	6.784	7.01
50	122	0.806	6.726	5.17
60	140	0.799	6.667	3.89
70	158	0.792	6.609	2.96
80	176	0.785	6.55	2.3
90	194	0.778	6.492	1.8
100	212	0.771	6.433	1.43
120	248	0.757	6.317	0.932
140	284	0.743	6.2	0.632
160	320	0.729	6.083	0.443
180	356	0.715	5.966	0.32
200	392	0.701	5.849	0.238

Equations:

Density: $d(\text{g/mL}) = 0.841 - 0.0007t$; $t = \text{°C}$

Viscosity: $\log_{10}(\text{cp}) = -3.7119 + 1532.19/(t + 296.2)$; $t = \text{°C}$

Experimental range: 25-100 °C

PHYSICAL PROPERTIES

Property	Value
Formula	(n-C ₆ H ₉) ₃ Al
Formula weight	198.33
State and color at 25°C	clear, colorless liquid
Stability in contact with air	fumes vigorously, may ignite spontaneously
Stability in contact with water	reacts violently
Melting point, °C	< -60
Boiling point at 760 mm Hg, °C	240 (464)
Vapor pressure, mm Hg at:	
40°C (104°F)	0.0041
60°C (140°F)	0.0358
80°C (176°F)	0.235
100°C (212°F)	1.20
120°C (248°F)	4.98
140°C (284°F)	16.7
160°C (320°F)	47.1
180°C (356°F)	113.2
200°C (392°F)	237.1
220°C (428°F)	443.0
240°C (464°F)	759.0
Specific heat at 20°C, cal/g°C	0.513
Specific heat at 68°F, btu/lb°F	0.513
Heat of vaporization at NBP, cal/g	60.53
Heat of vaporization at NBP, btu/lb	109
ΔH° of formation at 25°C, kcal/gfw	-80.8
Heat of combustion, net at 25°C, cal/g	10223
Heat of combustion, net at 77°F, btu/lb	994
Heat of reaction with water at 25°C, cal/g	552
Heat of reaction with water at 77°F, btu/lb	994
Coefficient of volume expansion at 25°C, per °C	0.000868
Decomposition rate¹ (%/min) at saturation pressure at:	
100°C (%/min)	0.00864
120°C (%/min)	0.0305
140°C (%/min)	0.120
160°C (%/min)	0.374
180°C (%/min)	1.05
200°C (%/min)	2.71
220°C (%/min)	4.26
240°C (%/min)	14.40

¹Equation: $\log_{10}(\%/min) = 9.747 - 4407/(t + 273.15)$; t = °C

Experimental range: 70 - 150°C

SAFETY & HANDLING

The pyrophoric nature of TNBA presents potential hazards not common to most liquid chemicals used by industry in tank truck quantities. TNBA, being pyrophoric, breaks into flame spontaneously and gives off dense smoke when exposed to air. It reacts violently with water. TNBA is a clear, non-corrosive mobile liquid with a low vapor pressure. Hydrocarbon solutions of TNBA, depending on the concentration and temperature, may not be pyrophoric. However, these solutions must still be blanketed with an inert gas such as dry nitrogen because TNBA 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-butylaluminum)
 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.

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