Technical Data Sheet
Date of Issue: 2026/09/03

TIBA
Triisobutylaluminum

CAS Number	100-99-2
EINECS/EC	202-906-3
Molecular Formula	$(i\text{-}C_4H_9)_3Al$

APPLICATION

Triisobutylaluminum (TIBA) is used primarily as a catalyst component in Ziegler-Natta type systems for olefin and diene polymerizations. Other applications include use as a reducing agent with selective activity in certain organic reduction reactions and as a chemical intermediate.

SPECIFICATION

Aluminum, wt %, min	13.4
TIBA, wt %, min	97
TNBA, wt %, max	0.5
Dissolved Isobutylene, wt %, max	2.5
Hydride (calculated as AlH_3), wt %, max	0.5

*Tends to increase during storage

STATISTICAL DATA

	Average ($\bar{x}$)	Variation (3σ)
Aluminum, wt %	13.7	0.2
TIBA, wt %	98.8	1.5
TNBA, wt %	0.04	0.24
Dissolved Isobutylene, wt %	0.6	1.2
Hydride (calculated as AlH_3), wt %	0.2	0.2

DENSITY & VISCOSITY

Temperature		Density		Viscosity
°C	°F	g/mL	lbs/gal	cp
10	50	0.7983	6.662	3.811
20	68	0.7876	6.573	2.301
25	77	0.7823	6.528	1.9
30	86	0.7769	6.484	1.619
40	104	0.7662	6.394	1.25
50	122	0.7555	6.305	1.024
60	140	0.7448	6.216	0.875
70	158	0.7341	6.126	0.77
80	176	0.7234	6.037	0.693
90	194	0.7127	5.948	0.634
100	212	0.702	5.858	0.588
110	230	0.6913	5.769	0.551
120	248	0.6806	5.68	0.52
130	266	0.6699	5.591	0.495
140	284	0.6592	5.501	0.473
150	302	0.6485	5.412	0.455

Equations:

Density: $d(g/mL) = 0.8090 - 0.00107t$; $t = °C$

Viscosity: $\log_{10}(cp) = -0.6457 + 56.432/(t + 36)$

Experimental range: 20 - 55°C

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PHYSICAL PROPERTIES

Property	Value
Property	$(i\text{-}C_4H_9)_3Al$
Formula weight	198.33
State and color at 25C	clear, colorless liquid
Stability in contact with air	fumes vigorously, may ignite spontaneously
Stability in contact with water	reacts violently
Freezing point, C (F)	1.0 (33.8)
Boiling point at 30 mm Hg, C (F)	113.8 (236.8)
Boiling point at 760 mm Hg, C (F)	212.4 (414.3)
Vapor pressure[1], mm Hg at:	
50C (122F)	0.92
70C (158F)	3.30
90C (194F)	10.00
100C (212F)	16.30
120C (240F)	34.50
140C (284F)	85.90
Specific heat at 68F	0.670 btu/lbF
Specific heat at 20C	0.670 cal/gC
Heat of vaporization at NBP	52.4 cal/g; 94.4 btu/lb
ΔH° of formation at 25C (77F)	-79.6 kcal/gfw
Heat of combustion, net at 25C	10,233 cal/g
Heat of combustion at 77F	18,427 btu/lb
Heat of reaction with water at 25C (77F)	589.4 cal/g
Surface tension at 25.2C (77.4F)	21.3 dyne/cm
Coefficient of volume expansion at 20C	0.00140/C
Critical temperature, C	383.49
Critical pressure, mmHg	13889
Decomposition rate[2] (%/minute) under reflux at:	
70C (158F)	0.105
90C (194F)	0.353
110C (230F)	1.070
130C (266F)	2.870
150C (302F)	7.000

[1]log P = 7.3470 - 1841.9/(t+200); t = °C, P = mm Hg
Experimental range = 55 - 90°C
[2]$\log_{10}$(% min) = 7.668 - 3314.6/(t+273.15); t = °C
Experimental range = 90 - 130°C

HANDLING & STORAGE

The pyrophoric nature of TIBA presents potential hazards not common to most liquid chemicals used by industry in tank truck quantities. TIBA, being pyrophoric, breaks into flame spontaneously and gives off dense smoke when exposed to air. It reacts violently with water. TIBA is a clear, non-corrosive mobile liquid with a low vapor pressure. Hydrocarbon solutions of TIBA, 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 TIBA 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

	Nominal Value		Approximate Loadings	
Container Description	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.....Aluminum Alkyl (Triisobutylaluminum)
Hazard class.....4.2 (spontaneously combustible)
ID number.....UN3051
Placard(s .....spontaneously combustible w/ number 4
Label(s.....spontaneously combustible
MARPOL Classification .....n/a
Harmonized tariff number 2931.00.4000-2
Schedule B number 2931.00.6000-7

OTHER INFORMATION

Further Related Documents — Safety Data Sheet

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