

DIBAC

Diisobutylaluminum chloride

CAS Number	1779-25-5
EINECS/EC	217-216-8
Molecular Formula	$(i-C_4H_9)_2AlCl$

APPLICATION

Diisobutylaluminum chloride (DIBAC) 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 %	15.0 - 15.5
Chlorine/Aluminum, atom ratio	1.00 - 1.05
Hydride (calculated as AlH_3), wt% max	0.07
Hydrolysis gas composition	
Ethane, mol %, min	1.4
n-Butane & Isobutane, mol %, max	0.5
Isobutane, mol %, max	97.5
Methane, mol %, max	0.5
Propane, mol %, max	0.5

STATISTICAL DATA

	Average (\bar{x})	Variation (3σ)
Aluminum, wt %	15.25	0.25
Iodine, wt %	-1.025	0.025
Methane, mol %	0.2	(*)
Hydrolysis gas composition		
Ethane, mol %	0.5	1.0
Propane, mol %	0.3	(*)
n-Butane & Isobutane, mol %	0.3	(*)
Isobutane, mol %	98.9	1.1

(*) Insufficient data to determine sigma.

DENSITY & VISCOSITY

Temperature		Density		Viscosity
°C	°F	g/mL	lbs/gal	cp
0	32	0.9319	7.776	7.88
10	50	0.9238	7.709	5.86
20	68	0.9158	7.642	4.49
25	77	0.9118	7.608	3.97
30	86	0.9078	7.575	3.53
40	104	0.8998	7.508	2.84
50	122	0.8918	7.441	2.33
60	140	0.8837	7.374	1.94
70	158	0.8757	7.307	1.64
80	176	0.8677	7.24	1.41
90	194	0.8597	7.173	1.22
100	212	0.8516	7.106	1.07
120	248	0.8356	6.973	0.85
140	284	0.8196	6.839	0.69
160	320	0.8035	6.705	0.57
180	356	0.7875	6.571	0.49
200	392	0.7714	6.437	0.42

Equations:

Density: $d(g/mL) = 0.9319 - 0.000803t$; $t = ^\circ C$

Viscosity: $\log_{10}(cp) = -1.4804 + 414.3/(t + 174.3)$; $t = ^\circ C$

Experimental range: 25 - 140°C

PHYSICAL PROPERTIES

Property	Value
Formula	(i-C ₄ H ₉) ₂ AlCl
Formula weight	176.67
State and color at 25°C	clear, colorless liquid
Stability in contact with air	fumes vigorously
Stability in contact with water	reacts violently
Melting Point °C (°F)	-40 (-40)
Boiling point at 760 mm Hg, °C (°F)	290 (554)
Vapor pressure, mm Hg at 0°C (32°F)	0.000042
Vapor pressure, mm Hg at 20°C (68°F)	0.000573
Vapor pressure, mm Hg at 40°C (104°F)	0.005054
Vapor pressure, mm Hg at 60°C (140°F)	0.03185
Vapor pressure, mm Hg at 80°C (176°F)	0.1541
Vapor pressure, mm Hg at 100°C (212°F)	0.6042
Vapor pressure, mm Hg at 120°C (248°F)	1.9957
Vapor pressure, mm Hg at 140°C (284°F)	5.716
Vapor pressure, mm Hg at 160°C (320°F)	14.367
Vapor pressure, mm Hg at 180°C (356°F)	32.334
Vapor pressure, mm Hg at 200°C (392°F)	66.396
Vapor pressure, mm Hg at 220°C (428°F)	126.24
Vapor pressure, mm Hg at 240°C (464°F)	224.86
Specific heat at 20°C, cal/g°C	0.426
Specific heat at 68°F, btu/lb°F	0.426
Heat of vaporization at NBP, cal/g, btu/lb	34.88 / 62.82
ΔH° of formation at 25°C, kcal/gfw	-119.5
Heat of combustion, net at 25°C, cal/g	-7,600
Heat of combustion, 77°F, btu/lb	13,681
Heat of reaction with water at 25°C, cal/g	-531
Heat of reaction with water, 77°F, btu/lb	956
Coefficient of volume expansion at 25°C, per/°C	0.000899
Critical pressure, atm	13.55
Critical temperature, °C	453.5

HANDLING & STORAGE

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

Hazard class4.2 (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 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

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