

## Boranes

CalSelect™ Na

MDEB

TEB

Calselect™ Li

STAB

(R)-MeCBS

TnBB

PinB

TEB-DAP

DEANB

(S)-M

CalSe

DM

TnBB-M

9-BE

Ts

B-T

## Bases

LiHMDS

KHMDS

Toluene or THF

Potassium t-butoxide  
(Potassium t-butylate)

NaHMDS

STB  
KDMO 50% Heptane  
Potassium Ethylate

Potassium Isopropoxide

## Specialty Boron Reagents and Organic Bases

Product Overview

# Enabling the World's Most Important Products from Lab Through Commercialization

At Callery, we enable our customer's success. From boranes to alkoxides, to custom organometallics, Callery's impressive combination of innovation, scale, customer service, and supply chain security gives us a distinct advantage. Our products have enabled some of the world's most successful innovations from billion-dollar blockbuster drugs to next-generation OLEDs.

## A CLEAR LEADER IN HIGHLY-REACTIVE REAGENTS

Our decades of experience and ability to produce highly reactive compounds that begin in our 50,000-ft<sup>2</sup> research and development lab to full production of multi tons of product. Combine this with our signature customer support, quality management system, and global logistics expertise, Callery understands what it truly means to de-risk your supply chain.



### Superior Quality and Performance

We continue to deliver high quality reagents, enabling our customer's downstream products and providing distinct advantages in terms of purity, yield, and overall performance. Our quality management system means strict adherence to procedures and a robust change control process.



### Unparalleled Customer Support

A hallmark of Callery has always been customer support. Our technical support staff has extensive experience in handling your most difficult challenges. Whether you need a fast response to questions on specifications, a change in packaging, or need on-site training on the safe handling of Boranes or other organometallics, our experts are there to make sure you are 100% satisfied.



### Safe Handling of Highly-Reactive Compounds at Any Scale

Callery's capabilities extend to a wide variety of highly reactive compounds including many organometallics, boranes, and alkoxides. Strict adherence to SOPs and advanced engineering controls means we can safely produce your highly-reactive products. And because we have a wide range of equipment, we can provide the appropriate batch size, leading to competitive pricing.



### Absolute Security of Supply and Global Rapid Delivery

Callery prides itself in not only providing a quality product, but providing a clear pathway to supply. Callery's North American location and strict adherence to quality, EHS, and ISO and EPA standards means we are in control of everything from incoming raw materials to shipping of your product. With significant global logistics expertise, including temperature-controlled storage and warehousing facilities in the US and EU, we ensure safe, secure and timely delivery of your orders.



### Impressive Innovation Engine

Callery hasn't become the world's number one supplier of alkoxides and boranes by chance. We amassed years of R&D into an extensive list of products, and have safely scaled many of them to 100s of tons. The size, scope and expertise in our R&D center can drive some of your most demanding challenges. Whether you are looking for a custom borane, alkoxide, or any other organometallic, we have the capabilities and expertise to make it happen.

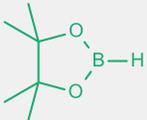
## DIVERSIFIED SPECIALTY CHEMICAL EXPERTS

Callery has developed a wide array of products, all stemming from a focus centered around the safe handling of highly-reactive molecules including boranes, alkoxides, and other organometallics. This focused expertise has resulted in Callery being a leading global supplier in all our product classes.

### Suzuki Coupling Reagents

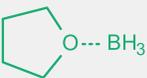
Boronic acids and esters have become very important building blocks in organic synthesis through the Suzuki-Miyaura cross-coupling protocols. The Suzuki-Miyaura reaction<sup>1</sup> is a powerful synthetic tool for the formation of carbon-carbon bonds, dramatically shortening multi-step synthetic routes since this process easily couples large molecular fragments containing functional groups. Trialkylborane and aryldialkylborane reagents can also participate in these valuable coupling reactions.

<sup>1</sup> Miyaura, N.; Suzuki, A. *Chem. Rev.* **1995**, *95*, 2457.

Name	Abbreviation / Trade Name	Structure	CAS#	Formula FW (g/mol)	Form	Density (g/ml)
Pinacolborane	PINB		25015-63-8	C <sub>6</sub> H <sub>13</sub> BO <sub>2</sub> 128.00	Neat w/ 1% TEA	0.875
9-Borabicyclo[3.3.1]nonane	9BBN		280-64-8	C <sub>8</sub> H <sub>15</sub> B 122.02	0.5M in THF	0.882

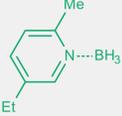
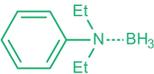
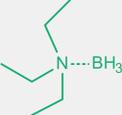
### Borane Complexes

Borane complexes are versatile compounds commonly used as regio-, chemo- and stereoselective reducing agents for a variety of functional groups such as aldehydes, ketones, carboxylic acids, amides and olefins. The high yields and simple isolation of the reduced products combined with the high selectivities achieved with borane reagents have made these compounds the preferred reducing agents for a number of applications.

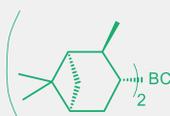
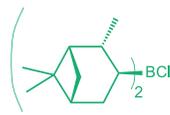
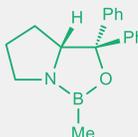
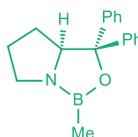
Name	Abbreviation / Trade Name	Structure	CAS#	Formula FW (g/mol)	Form	Density (g/ml)
Borane tetrahydrofuran complex	BTHF		14044-65-6	C <sub>4</sub> H <sub>11</sub> BO 85.94	1M in THF	0.878
Dimethylsulfide borane complex	DMSB		13292-87-0	C <sub>2</sub> H <sub>9</sub> BS 75.97	10M in DMS	0.794

## Amine Boranes

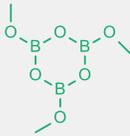
Complexation of borane with a strong Lewis base, such as an unhindered amine, produces air and moisture stable amine borane complexes. The stability, solubility, and ease of handling make them attractive borane sources in many reactions where aqueous, alcoholic or acidic solvents are desirable. 5-Ethyl-2-methylpyridine borane is a new complex which is easily handled and has up to three hydrides available for reductive amination and reduction.

Name	Abbreviation / Trade Name	Structure	CAS#	Formula FW (g/mol)	Form	Density (g/ml)
5-Ethyl-2-methylpyridine borane	PEMB		1006873-58-0	C <sub>8</sub> H <sub>14</sub> BN 135.01	Neat Liquid	0.913
N,N-Diethylaniline borane	DEANB		13289-97-9	C <sub>10</sub> H <sub>18</sub> BN 163.07	Neat Liquid	0.921
Triethylamine borane	TEAB		1722-26-5	C <sub>6</sub> H <sub>18</sub> BN 115.03	Neat Liquid	0.782

## Chiral Reagents

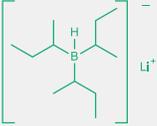
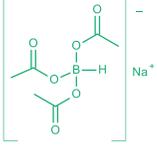
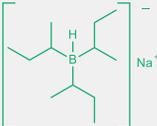
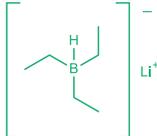
Name	Abbreviation / Trade Name	Structure	CAS#	Formula FW (g/mol)	Form	Density (g/ml)
(-)-Diisopinocampheylchloroborane	(-)-DPC		85116-37-6	C <sub>20</sub> H <sub>34</sub> BCl 320.80	60-65 wt% heptanes	0.828
(+)-Diisopinocampheylchloroborane	(+)-DPC		112246-73-8	C <sub>20</sub> H <sub>34</sub> BCl 320.80	60-65 wt% hexanes	0.860
(R)-Methyl oxazaborolidine	(R)-MeCBS		112022-83-0	C <sub>18</sub> H <sub>20</sub> BNO 277.17	1M in toluene	0.927
(S)-Methyl oxazaborolidine	(S)-MeCBS		112022-81-8	C <sub>18</sub> H <sub>20</sub> BNO 277.17	1M in toluene	0.927

## Boroxine

Name	Abbreviation / Trade Name	Structure	CAS#	Formula FW (g/mol)	Form	Density (g/ml)
Trimethoxyboroxin	TMBX		102-24-9	C <sub>3</sub> H <sub>9</sub> B <sub>3</sub> O <sub>6</sub> 173.53	Neat liquid	1.216
Trimethylboroxin	MBX		823-96-1	C <sub>3</sub> H <sub>9</sub> B <sub>3</sub> O <sub>3</sub> 125.53	50 wt% in THF	0.894

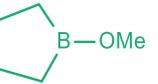
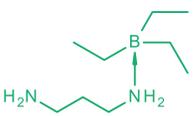
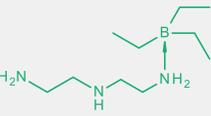
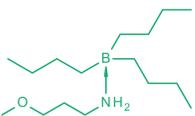
## Calselect® Reducing Agents

Alkali metal trialkylborohydrides have been used in numerous stereoselective and regioselective reductions. The strength and reactivity of these reducing agents varies with the steric bulk of the alkyl groups and the alkali metal ion. Calselect® STAB is a selective reducing agent that has proven to be extremely useful in reductive aminations.

Name	Abbreviation / Trade Name	Structure	CAS#	Formula FW (g/mol)	Form	Density (g/ml)
Lithium tri- <i>sec</i> -butylborohydride	CALSELECT® Li		38721-52-7	C <sub>12</sub> H <sub>28</sub> BLi 190.11	1M in THF	0.898
Sodium triacetoxymethylborohydride	CALSELECT® STAB		56553-60-7	C <sub>6</sub> H <sub>10</sub> BNaO <sub>6</sub> 211.96	Powder Granular	0.765
Sodium tri- <i>sec</i> -butylborohydride	CALSELECT® Na		67276-04-4	C <sub>12</sub> H <sub>28</sub> BNa 206.15	1M in THF	0.898
Lithium triethylborohydride	CALSELECT® LT		22560-16-3	C <sub>6</sub> H <sub>16</sub> BLi 105.95	1M in THF	0.890

## Alkylboranes

Alkylboranes are versatile products used in different industrial applications such as Pharmaceuticals, Polymers and others. In organic synthesis triethylborane (TEB) and methoxydiethylborane (MDEB) have proven especially effective as diastereoselective reagents to produce *syn*-diols from  $\beta$ -hydroxyketones.

Name	Abbreviation / Trade Name	Structure	CAS#	Formula FW (g/mol)	Form	Density (g/ml)
9-Borabicyclo[3.3.1]nonane	9BBN		280-64-8	C <sub>8</sub> H <sub>15</sub> B 122.02	0.5M in THF	0.882
Methoxydiethylborane	MDEB		7397-46-8	C <sub>5</sub> H <sub>13</sub> BO 99.97	Neat liquid 50 wt% in THF	0.749 0.807
Triethylborane	TEB		97-94-9	C <sub>6</sub> H <sub>15</sub> B 98.00	Neat liquid 14 wt% in THF	0.696 0.848
Triethylborane-1,3-diaminopropane complex	TEB-DAP		1448861-07-8	C <sub>9</sub> H <sub>25</sub> BN <sub>2</sub> 172.12	Neat liquid	0.859
Triethylborane-Diethylenetriamine Complex	TEB-DETA		1187733-83-0	C <sub>10</sub> H <sub>28</sub> BN <sub>3</sub> 201.18	Liquid	0.890
Tri- <i>n</i> -butylborane-3-methoxypropylamine complex	TnBB-MOPA		345269-15-0	C <sub>15</sub> H <sub>37</sub> BNO 271.25	Neat liquid	0.826



## Alkali Metal Alkoxides

Alkoxides are moderately strong base reagents that are used in many drug and chemical synthesis applications, such as alkylation, arylation, acylation, solvolysis of esters, condensation, elimination, isomerization, rearrangements, transfer, hydrogenation, Wittig reactions, and redox reactions. The reactivity can be fine tuned to the desired reaction by correct choice of alkali metal and counterion. The wide range of properties and solubilities available from Callery allows for process optimization and high yields.

### Potassium Alkoxides

Name / Synonym	Abbreviation / Trade Name	Structure	CAS#	Formula FW (g/mol)	Form	Density (g/ml)
Potassium 3,7-Dimethyl-3-octylate <i>Potassium 3,7-Dimethyl-3-octanoxide</i>	KDMO/Heptane 50%		263148-42-1	$C_{10}H_{21}KO$ 196.37	50% w/w in n-heptane	0.804
Potassium Ethylate <i>Potassium Ethoxide</i>	KE 24% (DN with toluene)		917-58-8	$C_2H_5KO$ 84.14	24% w/w in ethanol	0.895
Potassium Iso-Propylate <i>Potassium Iso-Propoxide</i>	KIP/IPA 19%		6831-82-9	$C_3H_7KO$ 98.19	19% w/w in isopropanol	0.862
Potassium tert.-Amylate <i>Potassium tert.-Pentoxide</i>	KTA/Cyclohexane 15% KTA/Toluene 25%		41233-93-6	$C_5H_{11}KO$ 126.20	15% w/w in cyclohexane 25% w/w in toluene	0.801 0.904
Potassium tert.-Butylate <i>Potassium tert-Butoxide</i>	KTB		865-47-4	$C_4H_9KO$ 112.21	Powder 20% w/w in THF	0.813 0.906

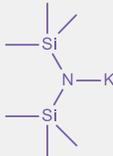
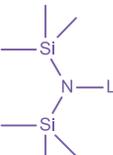
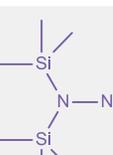
### Sodium Alkoxides

Name / Synonym	Abbreviation / Trade Name	Structure	CAS#	Formula FW (g/mol)	Form	Density (g/ml)
Sodium Mentholate	NaM/Hexanes 50%		1321-38-1	$C_{10}H_{19}NaO$ 178.25	50% w/w in hexanes	0.815
Sodium tert.-Amylate <i>Sodium tert.-Pentoxide</i>	STA STA/THF 35%		14593-46-5	$C_5H_{11}NaO$ 110.13	Powder 35% w/w in THF	0.926
Sodium tert.-Butylate <i>Sodium tert-Butoxide</i>	STB		865-48-5	$C_4H_9NaO$ 96.02	Powder	0.698



## Alkali Metal Amides

Potassium hexamethyldisilazane (KHMDS), sodium hexamethyldisilazane (NaHMDS), and lithium hexamethyldisilazane (LiHMDS) are strong non-nucleophilic base reagents useful in a wide variety of chemical reactions and transformations. Applications include alkylation acylation, ring formation, isomerization, rearrangements, aldol condensations, Wittig and Horner-Emmons reactions and polymerization. Their high selectivity and specificity can lead to simpler, less expensive purification routes to the desired product.

Name / Synonym	Abbreviation / Trade Name	Structure	CAS#	Formula FW (g/mol)	Form	Density (g/ml)
Potassium Hexamethyldisilazane <i>Potassium bis(trimethylsilyl)amide</i>	KHMDS/ Toluene 15%		40949-94-8	$C_6H_{18}KNSi_2$ 199.5	15% w/w in toluene	0.879
Lithium Hexamethyldisilazane <i>Lithium bis(trimethylsilyl)amide</i>	LiHMDS/ THF 24%		4039-32-1	$C_6H_{18}LiNSi_2$ 167.33	24% w/w in THF	0.867
Sodium Hexamethyldisilazane <i>Sodium bis(trimethylsilyl)amide</i>	NaHMDS/ THF 40%		1070-89-9	$C_6H_{18}NNaSi_2$ 183.38	40% w/w in THF	0.889

## Other Alkali Metal Compounds

Sodium-Potassium Alloy (NaK), essentially a liquid form of Potassium metal, is mainly used for reductions and as a raw material for making potassium derivatives. Potassium superoxide ( $KO_2$ ) has its main applications as a chemical oxygen source.

Name / Synonym	Abbreviation / Trade Name	Structure	CAS#	Formula FW (g/mol)	Form	Density (g/ml)
Potassium Superoxide	$KO_2$ UNCAT fluff	$KO_2$	12030-88-5	$KO_2$	Uncatalyzed fluff	0.16-0.320 g/cc
Sodium Potassium Alloy	NaK	NaK	11135-81-2	NaK	Liquid	0.855
Potassium Metal	K-Metal	K	7440-09-7	K	Easily melted solid	0.862

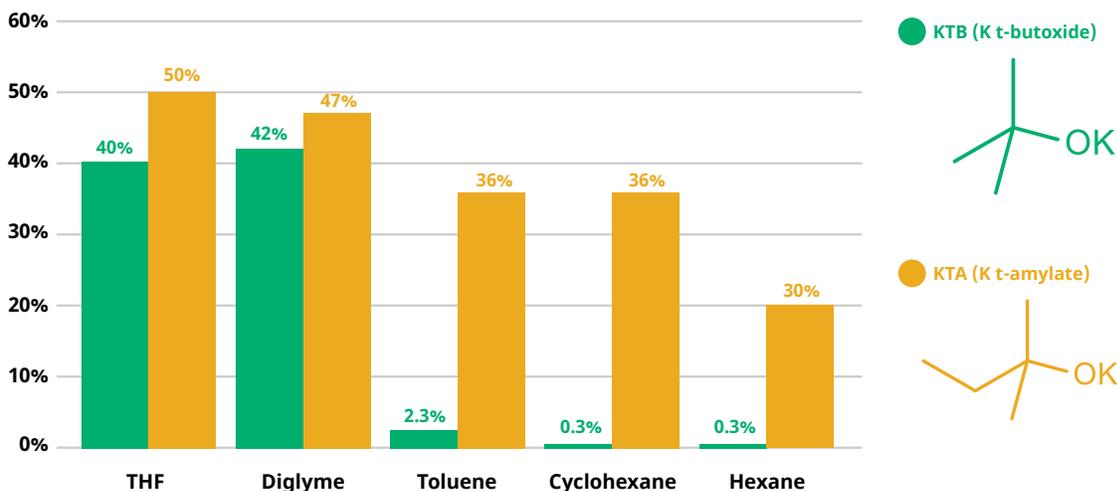
## Selectivity of Callery's Boron Reducing Agents

	Aldehyde	Imine	Ketone	Epoxide	Nitrile	Carboxylic acid	2° - amide	Olefin	Acid Halide	Lactone	Ester	Alkyl Halide	Nitro
BTHF	●	●	●	●	●	●	●	●	●	●	●	●	●
DMSB	●	●	●	●	●	●	●	●	●	●	●	●	●
DEANB	●	●	●	●	●	●	●	●	●	●	●	●	●
CalSelect® Li	●	●	●	●	●	●	●	A	●	●	●	●	●
CalSelect® Na	●	●	●	●	●	●	●	A	●	●	●	●	●
CalSelect® Lt	●	●	●	G	H	●	I	A	●	●	●	●	●
TEAB	●	●	●	●	●	E	●	F	●	●	●	●	●
PEMB	●	●	●	●	●	D	●	●	●	●	●	●	●
CalSelect® STAB	●	●	B	●	●	●	●	C	●	●	●	●	●

● Reduction reaction  
 ● No reaction  
 ● Special case

A enones  
 B β-hydroxyketones only  
 C enamines, guanolines, indoles  
 D with BF<sub>3</sub>  
 E at 80°C, neat  
 F high temperature  
 G Markovnikov, alcohol only  
 H aromatic nitriles only  
 I tertiary amides are reduced

## Potassium Alkoxide Solubility (25°C)



The data contained in this publication is based on our current knowledge and experience. In view of the many factors that may affect processing and application of our product, the data does not relieve processors from carrying out their own investigations and tests; neither does the data imply any guarantee of certain properties, nor the suitability of the product for a specific purpose. Any descriptions, drawings, photographs, data, proportions, weights etc. given herein may change without prior information and do not constitute the agreed contractual quality of the product. It is the responsibility of the recipient of our products to ensure that any proprietary rights and existing laws and legislation are observed. The safety data given in this publication is for information purposes only and does not constitute a legally binding Safety Data Sheet (SDS). The relevant SDS can be obtained upon request from your supplier or you may contact Callery directly at [customer.care@callery.com](mailto:customer.care@callery.com)



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