

# TECHNICAL DATA SHEET

Date of Issue: 2017/01/09

## Zinc Chloro 2,2,6,6-Tetramethylpiperidide Lithium Chloride Complex, typ. 17 % solution in THF (typ. 0.7 M)

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Molecular Formula  $C_9H_{18}ClZnN \cdot LiCl$

Product Number 408613

### APPLICATION

Selective deprotonation of arenes and heteroarenes.

Arenes and heteroarenes are typically deprotonated by a directed lithiation using organolithium compounds or organolithiumamides (e.g. LDA). The high reactivity and nucleophilicity of these reagents often result in unwanted side reactions and precludes the presence of sensitive functional groups like esters or ketones. Additionally, such deprotonation reactions often require low temperatures leading to higher production costs on larger scale.

Due to their low kinetic basicity zinc-amides tolerate a lot of functional groups.

### FURTHER INGREDIENTS

Tetrahydrofuran

CAS-No. 109-99-9

EC-No. 203-726-8

Zinc chloro 2,2,6,6-tetramethylpiperidide lithium chloride complex (1:1)

CAS-No. 1145881-09-9

EC-No. not registered

Lithium chloride

CAS-No. 7447-41-8

EC-No. 231-212-3

### SPECIFICATION

active base as TMP-ZnCl 16.0 - 18.5 %

w/o LiCl

Zn 0.80 - 0.95 mmol/g

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molar ratio Zn/Li 0.9 – 1.1

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## METHOD OF ANALYSIS

Active base: Titration with benzoic acid (modified Watson-Eastham titration). Detailed description is available on request.

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## PHYSICAL PROPERTIES

Appearance	liquid
Color	brownish clear to cloudy
Flash point	-21.2 °C (Tetrahydrofuran)
Boiling point/boiling range	66 °C (Tetrahydrofuran)
Density	0.95 g/cm <sup>3</sup> at 20 °C
Water solubility	(Not applicable)
Molecular weight	283.51 g/mol
Thermal Stability	decomposition above 20°C
Additional Physical Properties	<u>Molecular weight:</u> TMP-ZnCl 241.11 g/mol LiCl 42.4 g/mol

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## HANDLING & STORAGE

Handling	Organozinc compounds should only be handled under inert gas (nitrogen or argon). Never add water, acids or oxidizing materials to the product. In case of fire use dry extinguishers on basis of sodium chloride or limestone powder. Never use water or CO <sub>2</sub> -extinguishers. Pay attention to official Safety regulations (see also: 'Transport regulations' and 'Marking').
Storage	Store in well ventilated areas in tightly closed containers. As material decomposes slowly above room temperature recommended storage temperature is below 20 °C.

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## TRANSPORT & PACKAGING

UN number 2924

ADR	Class: 3	PG: II	Label: 3 (8)
RID	Class: 3	PG: II	Label: 3 (8)
IMDG	Class: 3	PG: II	Label: 3 (8)
IATA_C	Class: 3	PG: II	Packing instruction (cargo aircraft): 363
IATA_P	Class: 3	PG: II	Packing instruction (passenger aircraft): 352

Hazard pictograms



Signal Word                      Danger

H&P Phrases                      See Safety Data Sheet

Labelling                              The labelling is according to EU-GHS classification ((EG) 1272/2008) and may vary in other countries. Please refer to the respective Safety Data Sheet for your country.

Packaging

Glass bottles of 100, 250, 500, and 1,000 ml. Steel bottles and containers with volumes of 7.4 l, 27 l, 127 l or 450 l. For safety reasons these are filled to a maximum of 90 %. Steels drums with 200 l net volume.

## OTHER INFORMATION

Further Related                      Safety Data Sheet

Documents

Our brochure(s)                      Lithium & Magnesium Amides

Remarks                              **References / Literature:**

T. Bresser, G. Monzon, M. Mosrin, P. Knochel, *Org. Process Res. Dev.* **2010**, 14, 1299

M. Mosrin, T. Bresser, P. Knochel, *Org. Lett.* **2009**, 11, 3406

T. Bresser, M. Mosrin, G. Monzon, P. Knochel, *J. Org. Chem.* **2010**, 75, 4686

F. Gosselin, S. J. Savage, N. Blaquiere, S. T. Staben, *Org. Lett.* **2012**, 14, 862

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