

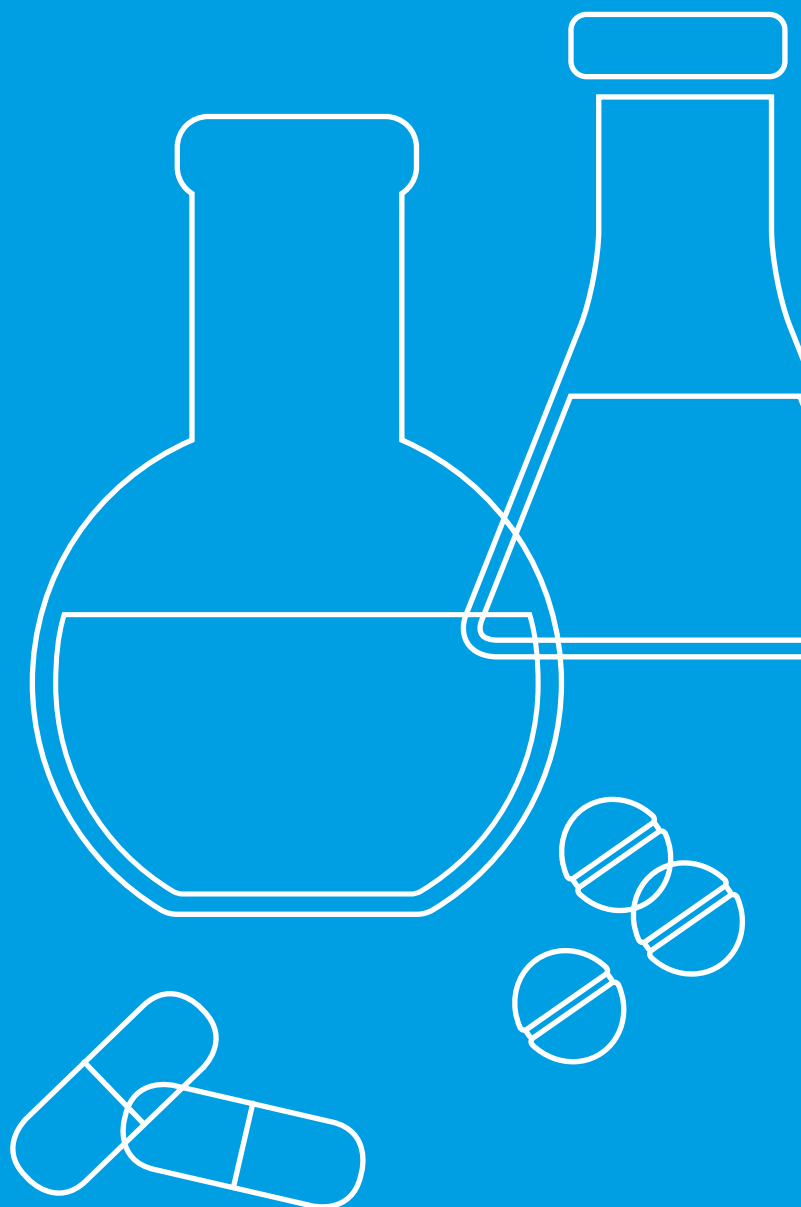


Better chemistry – achieving more.

# ALLESSAN<sup>®</sup> CAP

Propane Phosphonic Acid Anhydride (PPA)

Empirical Formula:  $[C_3H_7O_2P]_3$   
Molecular Weight: 318.18 g/mol  
CAS-No.: 68957-94-8



# ALLESSAN<sup>®</sup>CAP

## Benefits

Allessan<sup>®</sup>CAP is an outstanding peptide coupling and water removal reagent, offering several advantages over many other traditional but hazardous coupling reagents such as DCC (toxic), HOBT (explosive), HBTU and PyBOP.

## Advantages of Allessan<sup>®</sup>CAP

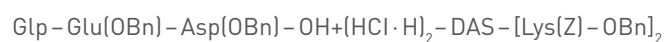
- Safe handling – no CMR properties, non-toxic, non-allergenic, non-sensitizing
- Excellent safety profile: high thermal stability, no decomposition
- Broad functional group tolerance, mild reaction conditions (0–25 °C)
- Well established at large scale for challenging liquid phase amide/peptide coupling reactions
- Low epimerization, no additives required
- Excellent selectivity, high chemical and optical purity, high product purities and excellent yields
- Easy purification/work up due to water soluble ionic by-products, no need of chromatographic columns
- Simple product isolation by liquid/liquid extraction and phase separation
- Reduced overall process costs
- Long shelf life (> 36 months)
- No special storage required

## Benefits of PPA versus common coupling reagents

| COUPLING REAGENT | TOXICITY  | EPIMERISATION | YIELD  | PURIFICATION   | COSTS     |
|------------------|-----------|---------------|--------|----------------|-----------|
| PPA              | no        | low           | high   | simple         | medium    |
| DCC              | high      | high          | low    | very difficult | low       |
| DCC/HOBT         | high      | medium        | medium | very difficult | low       |
| EDC              | high      | medium        | medium | simple         | medium    |
| BOP              | very high | low           | high   | difficult      | high      |
| PyClon           | medium    | low           | high   | difficult      | very high |
| TBTU/HBTU        | medium    | low           | high   | difficult      | medium    |

## Comparison of degree of racemization of different coupling reagents

| COUPLING REAGENT | RACEMIZATION [%] | YIELD [%] |
|------------------|------------------|-----------|
| PPA              | 1.8              | 86.6      |
| HOBT/DCC         | 5.9              | 60.5      |
| HOBT/EDC         | 11.1             | 67.3      |
| HOAt/DCC         | 11.6             | n. a.     |
| PyBOP            | 14.2             | 63.4      |
| HBTU             | 16.1             | 65.6      |
| HATU             | 21.1             | n. a.     |



## Applications

Allessan®CAP is a pH neutral dehydration reagent, similar in strength to the highly reactive and hazardous phosphorous pentoxid and polyphosphoric acid, alternative to molecular sieves for water removal from organic solvents and providing Lewis acid catalysis potential for reactions.

Thanks to its less toxic nature, broad spectrum of applications, high selectivity and mild operating conditions, Allessan®CAP offers several benefits in both medicinal chemistry and process chemistry.

## Allessan®CAP can be used for

- Peptide couplings (linear and cyclic peptides)
- Amidations
- Esterifications
- Functional Group Transformation (nitrile formation, olefine formation, alcohol oxidation, reduction of carboxylic acids, Lossen rearrangement, Beckmann rearrangement)
- Synthesis of heterocyclic compounds (pyrazolone, indole, quinolines, coumarins)
- Swern-type oxidations as a substitute of oxalyl dichloride and triethylamine
- Aza-Diels-Alder reactions as a catalyst

## Facility, Packaging and Solvents

### Facility

- Allessan®CAP has been produced for many years in an ISO9001 certified facility
- Capacity: several hundreds of tons per year

### Packaging

- 5 L, 50 L, 200 L steel drums with PE liners or twinlock drums (DMF)
- Only 5 L drums are allowed to be shipped by air freight

### Variety of Solvents

- Allessan®CAP is typically offered as a concentrated 50 % (w/w) solution in various kinds of solvents
- The most common solvents are EtOAc and THF, but we are highly flexible regarding our customer needs (DMF, 2-Me-THF, ACN, BuOAc, toluene, ...)

## Specification and Analytical Data

| NO. | QUALITY CHARACTERISTICS / PARAMETER / CONTENT      | ANALYTICAL METHOD | UNIT  | SPECIFIED VALUE / AREA | REMARKS |
|-----|--|-------------------|-------|------------------------|---------|
| 1   | Appearance   | visual            | -     | clear solution         | CoA     |
| 2   | Active content                                     | Calculation       | % m/m | min. 50                | CoA     |
| 3   | Solvent content                                    | GC                | % m/m | 40 – 44.5              | CoA     |
| 4   | Content of solvent free Allessan®CAP*              | Calculation       | % m/m | 55.5 – 60              | CoA     |
| 5   | Hydrogen chloride content of Allessan®CAP solution | IC                | %     | < 0.1                  | Inf     |

\* Content of solvent free Allessan®CAP = 100 – solvent content



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