

Allessan[®] CAP

Propane Phosphonic Acid Anhydride (PPA)

Benefits

Allessan[®] CAP is an outstanding coupling and water removal reagent, offering several advantages over many other commonly used but hazardous coupling reagents such as DCC (toxic), HOBt (explosive), HBTU or PyBOP.

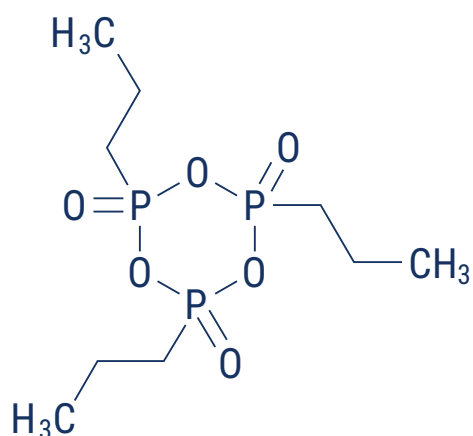
Advantages of Allessan[®] CAP

- 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 / easy work-up due to water soluble by-products, no need of further purifications.
- 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

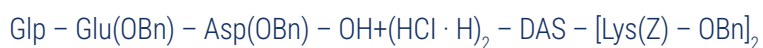
Coupling Reagent	Toxicity	Epimerisation	Yield	Purification	Costs
PPA	no	low	high	simple	medium
DCC	high	high	low	very difficult	low
DCC/HOBt	high	medium	medium	very difficult	low
EDC	high	medium	medium	simple	medium
BOP	very high	low	high	difficult	high
PyClop	medium	low	high	difficult	very high
TBTU/HBTU	medium	low	high	difficult	medium



Empirical Formula: C₃ H₇ O₂ P₃
CAS-No.: 68957-94-8
Molecular Weight: 318.18 g/mol

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.



PPA, DMF
DIPEA



Applications

Allessan[®] CAP is a pH neutral dehydration reagent, similar in strength to the highly reactive and hazardous phosphorous pentoxide 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 properties, broad spectrum of applications, high selectivity and mild operating conditions, Allessan[®] CAP offers several benefits in both medicinal chemistry and chemical processes.

Allessan[®] CAP can be used for:

- Peptides coupling (linear and cyclic peptides).
- Amidations.
- Esterifications.
- Functional group transformation (nitrile formation, olefin formation, alcohol oxidation, reduction of carboxylic acid, Lossen or Beckmann rearrangement).
- Synthesis of heterocyclic compounds (pyrazolones, indoles, quinolines, coumarins).
- Swern type oxidations as a substitute of oxalyl chloride and triethylamine.
- Aza-Diels-Alder reactions as a catalyst.



Facility and Packaging

- Allessan[®] CAP is 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.
- Ethyl acetate and THF are the most widely used, however, Allessan[®] CAP can be available in many other solvents (DMF, 2-Me-THF, Acetonitrile, Dichloromethane, 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



WeylChem Allessa GmbH

Alt-Fechenheim 34, 60386, Frankfurt / Main, Germany

Phone: +49 157 8061 7234

E-Mail: services@weylchem.com

www.weylchem.com

This data sheet does not constitute any representation or warranty and may not be treated as an offer to supply Product. We would be pleased to provide you a binding offer to supply Product meeting your individual needs and requirements.