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Better chemistry – achieving more.

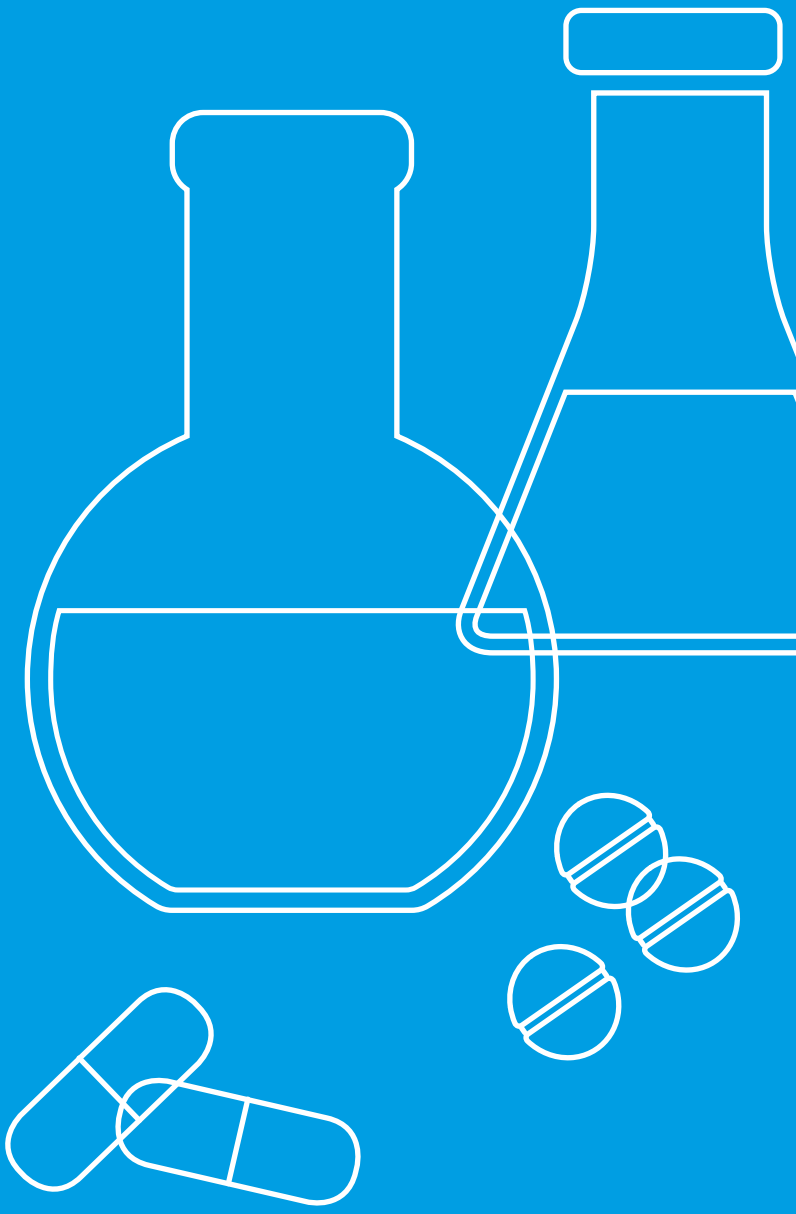
ALLESSAN®CAP

Propane Phosphonic Acid Anhydride (PPA)

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

Benefits

Allessan®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.



ALLESSAN®CAP

Advantages of Allessan®CAP

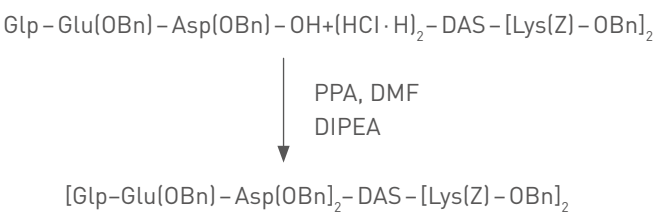
- Safe handling – no CMR properties, non-toxic, non-allergenic, non-sensitizing
- Excellent safety profile: high thermal stability, no decomposition
- Broad functional group tolerance, mild reaction conditions (0 –25 °C)
- Well established at large scale for challenging liquid phase amide/peptide coupling reactions
- Low epimerization, no additives required
- Excellent selectivity, high chemical and optical purity, high product purities and excellent yields
- Easy purification/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
PyClop	medium	low	high	difficult	very high
TBTU/HBTU	medium	low	high	difficult	medium

Comparision 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 strenghth 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, aclohol 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 inliners 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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