



>>Entry Name: Arsenobetaine

ENTRY UNDER REVIEW

Synonym(s): (Carboxymethyl)trimethylarsonium hydroxide inner salt, 9Cl

CAS Registry Number: 64436-13-1



Molecular Formula: C₅H₁₁AsO₂

Molecular Weight: 178.062

Accurate Mass: 177.997499

Percentage Composition: C 33.73%; H 6.23%; As 42.08%; O 17.97%

Source/Synthesis: Constit. of *Panulirus longipes cygnus*. Found in algae, lobsters, sharks, etc. Metab of (2-Hydroxyethyl)trimethylarsonium(1+) [FKN16-O](#). Not produced in mammals

Physical Description: Deliquescent cryst. (Me₂CO/MeOH)

Melting Point: Mp 204-210 dec.°

Other Data: Low mammalian toxicity, excreted unchanged e.g. from seafood sources.

Hazard & Toxicity: LD₅₀ (mus, orl) 10000 mg/kg

>>Derivative: Hydrobromide

CAS Registry Number: 71642-15-4

Molecular Formula: C₅H₁₂AsBrO₂

Molecular Weight: 258.974

Accurate Mass: 257.94366

Percentage Composition: C 23.19%; H 4.67%; As 28.93%; Br 30.85%; O 12.36%

Source/Synthesis: Synth. from AsMe₃ + BrCH₂COOH in toluene at 5° followed by stirring for 6 h then cooling (–20°; 30 min.)

Physical Description: Non-hygroscopic white shiny cryst. (EtOH, 5°)

References:

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Hanaoka, K. *et al.*, *Appl. Organomet. Chem.*, 1988, **2**, 371, (*occur, metab*)
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Siu, K.W.M. *et al.*, *Rapid Commun. Mass Spectrom.*, 1988, **2**, 69, (*ms*)
Beauchemin, D. *et al.*, *J. Anal. At. Spectrom.*, 1989, **4**, 285, (*hplc, ms*)
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Minhas, R. *et al.*, *Appl. Organomet. Chem.*, 1998, **12**, 635-641, (*synth, pmr, cmr, ms*)