



>>Entry Name: Mono(1,2,2-trimethylpropyl) methylphosphonate, 9CI

Synonym(s): Pinacolyl methylphosphonate

CAS Registry Number: 616-52-4

$(\text{H}_3\text{C})_3\text{CCH}(\text{CH}_3)\text{OPO}(\text{OH})\text{Me}$

Molecular Formula: $\text{C}_7\text{H}_{17}\text{O}_3\text{P}$

Molecular Weight: 180.183

Accurate Mass: 180.091532

Percentage Composition: C 46.66%; H 9.51%; O 26.64%; P 17.19%

Use/Importance: Metabolite and hydrol. product of Soman [DRM96-I](#). Chemical marker for compliance with chemical weapons treaties

Boiling Point: Bp₈ 96-106°

Density: d 1.03

pKa Value: pK_a 4.3 (20°, dioxan aq.)

Refractive Index: n_D²⁰ 1.4369

References:

Christol, H. *et al.*, *J. Organomet. Chem.*, 1968, **12**, 459-470, (*synth, ir, pmr, pKa*)

Reynolds, M.L. *et al.*, *Toxicol. Appl. Pharmacol.*, 1985, **80**, 409-420, (*metab*)

Soederstroem, M.T. *et al.*, *J. Chromatogr., A*, 1996, **742**, 191-203, (*anal*)