Figure S 1. RDFs for phosphorus-phosphorus interactions for (a) the NPT simulation and (b) the NVT simulation for all concentrations of TBP in dodecane.

Figure S . RDFs for sp2 oxygen-phosphorus interactions for (a) the NPT simulation and (b) the NVT simulation for all concentrations of TBP in dodecane.

Figure S . Diffusion constants for the NPT simulation of TBP in dodecane at various concentrations. These can be compared to results for the NVT simulation in the main paper.

Figure S . Enthalpy as a function of concentration for the NPT simulation of TBP in dodecane at various concentrations. These can be compared to results for the NVT simulation in the main paper.

Figure S . Screenshots of 20% TBP by volume in dodecane for (a) the NVT simulation and (b) the NP**T** simulation.

Figure S . Results for all concentrations collected using the in-house code from the NPT simulation. (a) Angle distributions and (b) Length distributions.