1-Phospha-1-butyne, 3,3-dimethyl-

Inchi: InChI=1S/C5H9P/c1-5(2,3)4-6/h1-3H3
InchiKey: PXQNAKPBTIQCTI-UHFFFAOYSA-N
Formula: C5H9P
SMILES: CC(C)(C)C#P
Mol. weight [g/mol]: 100.10
CAS: 78129-68-7

Physical Properties

Property code	Value	Unit	Source
ie	9.50	eV	NIST Webbook
ie	9.70	eV	NIST Webbook
log10ws	1.19		Crippen Method
logp	2.402		Crippen Method
mcvol	93.170	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C78129687&Units=SI

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume