2-Phosphapropene

Inchi: InChI=1S/C2H5P/c1-3-2/h1H2,2H3
InchiKey: ACYFLOXTAUSYGF-UHFFFAOYSA-N
Formula: C2H5P
SMILES: C=PC
Mol. weight [g/mol]: 60.03
CAS: 89149-01-9

Physical Properties

Property code	Value	Unit	Source
ie	9.50	eV	NIST Webbook
ie	9.69	eV	NIST Webbook
log10ws	3.01		Crippen Method
logp	0.994		Crippen Method
mcvol	55.200	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C89149019&Units=SI
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

Legend

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