1,3,2-Diazaphosphol-4-ene, 2-ethyl-2-oxo-1,3-dibutyl-4,5-dimethyl-

Inchi: InChI=1S/C14H29N2OP/c1-6-9-11-15-13(4)14(5)16(12-10-7-2)18(15,17)8-3/h6-12H2,1-5

InchiKey: XFRDMMKKZHCHBF-UHFFFAOYSA-N

Formula: C14H29N2OP

SMILES: CCCCN1C(C)=C(C)N(CCCC)P1(=O)CC

Mol. weight [g/mol]: 272.37

CAS: 104728-29-2

Physical Properties

Property code	Value	Unit	Source
ie	6.86	eV	NIST Webbook
log10ws	-5.84		Crippen Method
logp	4.669		Crippen Method
mcvol	239.250	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C104728292&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.