1,3,2-Diazaphosphol-4-ene, 2-(diethylamino)-1,3-dibutyl-4,5-dimethyl-

Inchi: InChI=1S/C16H34N3P/c1-7-11-13-18-15(5)16(6)19(14-12-8-2)20(18)17(9-3)10-4/h7-14H

InchiKey: CJZGXIOPBHLKHK-UHFFFAOYSA-N

Formula: C16H34N3P

SMILES: CCCCN1C(C)=C(C)N(CCCC)P1N(CC)CC

Mol. weight [g/mol]: 299.44

CAS: 141968-98-1

Physical Properties

Property code	Value	Unit	Source
ie	6.14	eV	NIST Webbook
log10ws	-1.79		Crippen Method
logp	5.024		Crippen Method
mcvol	271.540	ml/mol	McGowan Method

Sources

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=C141968981&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.