

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

Inchi:	InChI=1S/C14H29N2P/c1-6-9-11-15-13(4)14(5)16(12-10-7-2)17(15)8-3/h6-12H2,1-5H3
InchiKey:	RQICHKCPZXJYEQ-UHFFFAOYSA-N
Formula:	C14H29N2P
SMILES:	CCCCN1C(C)=C(C)N(CCCC)P1CC
Mol. weight [g/mol]:	256.37
CAS:	106054-01-7

Physical Properties

Property code	Value	Unit	Source
ie	6.60	eV	NIST Webbook
log10ws	-1.40		Crippen Method
logp	4.787		Crippen Method
mcvol	233.380	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106054017&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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