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
logp	2.402		Crippen Method
mcvol	93.170	ml/mol	McGowan Method
tf	234.22	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C78129687&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

Latest version available from:

https://www.chemeo.com/cid/68-941-2/1-Phospha-1-butyne-3-3-dimethyl.pdf

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