

Phosphirane

Inchi: InChI=1S/C2H5P/c1-2-3-1/h3H,1-2H2
InchiKey: UTMQOVWWMLZKRY-UHFFFAOYSA-N
Formula: C2H5P
SMILES: C1CP1
Mol. weight [g/mol]: 60.03
CAS: 6569-82-0

Physical Properties

Property code	Value	Unit	Source
affp	802.50	kJ/mol	NIST Webbook
basg	768.30	kJ/mol	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.40 ± 0.10	eV	NIST Webbook
log10ws	3.40		Crippen Method
logp	0.678		Crippen Method
mcvol	48.640	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C6569820&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

affp: Proton affinity
basg: Gas basicity
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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