Phosphine oxide, tri(1-methylethyl)

Other names:	((CH3)2CH)3P=O
	(i-C3H7)3PO
Inchi:	InChI=1S/C9H21OP/c1-7(2)11(10,8(3)4)9(5)6/h7-9H,1-6H3
InchiKey:	GEZGQQFKEOIGJS-UHFFFAOYSA-N
Formula:	C9H21OP
SMILES:	CC(C)P(=O)(C(C)C)C(C)C
Mol. weight [g/mol]:	176.24
CAS:	17513-58-5

Physical Properties

Property code	Value	Unit	Source
affp	954.40	kJ/mol	NIST Webbook
basg	924.50	kJ/mol	NIST Webbook
log10ws	-4.22		Crippen Method
logp	3.575		Crippen Method
mcvol	164.000	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17513585&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

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume