

PHOSPHINE OXIDE, TRIS(1-METHYLETHYL)-

Other names:	((CH ₃) ₂ CH) ₃ P=O (i-C ₃ H ₇) ₃ PO
Inchi:	InChI=1S/C ₉ H ₂₁ OP/c1-7(2)11(10,8(3)4)9(5)6/h7-9H,1-6H3
InchiKey:	GEZGQQFKEOIGJS-UHFFFAOYSA-N
Formula:	C ₉ H ₂₁ OP
SMILES:	CC(C)P(=O)(C(C)C)C(C)C
Mol. weight [g/mol]:	176.24

Physical Properties

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

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17513585&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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