PHOSPHORIC ACID, TRIS(1-METHYLETHYL) ESTER

Other names: Phosphoric acid, tris(1-methylethyl) ester
Isopropyl phosphate, (C3H7O)3PO
Phosphoric acid, triisopropyl ester

Inchi: InChI=1S/C9H21O4P/c1-7(2)11-14(10,12-8(3)4)13-9(5)6/h7-9H,1-6H3

InchiKey: OXFUXNFMHFCELM-UHFFFAOYSA-N

Formula: C9H21O4P

SMILES: CC(C)OP(=O)(OC(C)C)OC(C)C

Mol. weight [g/mol]: 224.24

Physical Properties

Property code	Value	Unit	Source
hvap	62.67	kJ/mol	Cheméo Relay (1.0)
logp	3.370		Crippen Method
mcvol	181.610	ml/mol	McGowan Method
rinpol	1182.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook

Sources

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):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C513020&Units=SI

Legend

hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices