

PHOSPHORIC ACID, TRIS(1-METHYLETHYL) ESTER

Other names:	Phosphoric acid, tris(1-methylethyl) ester Isopropyl phosphate, (C ₃ H ₇ O) ₃ PO Phosphoric acid, triisopropyl ester
Inchi:	InChI=1S/C ₉ H ₂₁ O ₄ P/c1-7(2)11-14(10,12-8(3)4)13-9(5)6/h7-9H,1-6H3
InchiKey:	OXFUXNFMHFCELM-UHFFFAOYSA-N
Formula:	C ₉ H ₂₁ O ₄ P
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

h_{vap}:	Enthalpy of vaporization at standard conditions
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
rin_{pol}:	Non-polar retention indices

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