

Triisobutyl phosphate

Other names:	phosphoric acid, triisobutyl ester phosphoric acid, tris(2-methylpropyl) ester
Inchi:	InChI=1S/C12H27O4P/c1-10(2)7-14-17(13,15-8-11(3)4)16-9-12(5)6/h10-12H,7-9H2,1-6H3
InchiKey:	HRKAMJBPFPHCSD-UHFFFAOYSA-N
Formula:	C12H27O4P
SMILES:	CC(C)COP(=O)(OCC(C)C)OCC(C)C
Mol. weight [g/mol]:	266.31
CAS:	126-71-6

Physical Properties

Property code	Value	Unit	Source
hvap	73.00	kJ/mol	NIST Webbook
hvap	76.30	kJ/mol	NIST Webbook
log10ws	-4.65		Crippen Method
logp	4.112		Crippen Method
mcvol	223.880	ml/mol	McGowan Method
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
tb	537.82	K	Estimation of Normal Boiling points of Trialkyl Phosphates using Retention indices by Gas Chromatography

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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hvapt	72.97	kJ/mol	298.15	Measurement of enthalpies of vaporization of trialkyl phosphates using correlation gas chromatography
hvapt	62.80	kJ/mol	474.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126716&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement of enthalpies of vaporization of trialkyl phosphates using correlation gas chromatography:	https://www.doi.org/10.1016/j.tca.2007.10.007
Estimation of Normal Boiling Point of Trialkyl Phosphates using Retention McGowan Method:	https://www.doi.org/10.1016/j.tca.2010.07.032
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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