tri-n-Amylphosphate

Other names:	phosphoric acid, tripentyl ester
	tri-n-pentyl phosphate
	triamyl phosphate
	tripentyl phosphate
Inchi:	InChI=1S/C15H33O4P/c1-4-7-10-13-17-20(16,18-14-11-8-5-2)19-15-12-9-6-3/h4-15H2,1
InchiKey:	QJAVUVZBMMXBRO-UHFFFAOYSA-N
Formula:	C15H33O4P
SMILES:	CCCCCOP(=O)(OCCCCC)OCCCCC
Mol. weight [g/mol]:	308.39
CAS:	2528-38-3

Physical Properties

Property code	Value	Unit	Source
hvap	92.30	kJ/mol	NIST Webbook
hvap	90.70	kJ/mol	NIST Webbook
log10ws	-6.63		Crippen Method
logp	5.715		Crippen Method
mcvol	266.150	ml/mol	McGowan Method
rinpol	1895.00		NIST Webbook
rinpol	1895.00		NIST Webbook
tb	596.36	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
hvapt	92.30	kJ/mol	298.15	Measurement of enthalpies of vaporization of trialkyl phosphates using correlation gas chromatography

srf	0.03	N/m	298.15	Strategy for extractant residual reduction: Experimental and computational investigation of fluorinated phosphate

Sources

Estimation of Normal Boiling points of Trialkyl Phosphates using Retention Indices by Gas Chromatography:	https://www.doi.org/10.1016/j.tca.2010.07.032
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2528383&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Strategy for extractant residual reduction: Experimental and computational investigation of fluorinated phosphate:	https://www.doi.org/10.1016/j.fluid.2017.06.026
Measurement of enthalpies of vaporization of trialkyl phosphates using correlation gas chromatography:	https://www.doi.org/10.1016/j.tca.2007.10.007

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
srf:	Surface Tension
tb:	Normal Boiling Point Temperature