TRIPENTYL PHOSPHATE

Other names: phosphoric acid, tripentyl ester
tri-n-pentyl phosphate
triamyl 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]: 308.40

Physical Properties

Property code	Value	Unit	Source
af	0.8404		Cheméo Relay (1.0)
hf	-1027.57	kJ/mol	Cheméo Relay (1.0)
hvap	92.30	kJ/mol	NIST Webbook
hvap	90.70	kJ/mol	NIST Webbook
ie	10.09	eV	Cheméo Relay (1.0)
log10ws	-4.14		Cheméo Relay (1.0)
logp	5.715		Crippen Method
mcvol	266.150	ml/mol	McGowan Method
pc	1514.82	kPa	Cheméo Relay (1.0, beta)
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
tc	730.44	K	Cheméo Relay (1.0)
tf	214.88	K	Cheméo Relay (1.0)
vc	1.038	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Strategy for extractant residual reduction: Experimental and computational investigation of fluorinated phosphate: https://www.doi.org/10.1016/j.fluid.2017.06.026

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2528383&Units=SI

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0, beta):

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 points of Trialkyl Phosphates using Retention indices by Gas Chromatography: https://www.doi.org/10.1016/j.tca.2010.07.032

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume