

Tripropyl phosphate

Other names:	phosphoric acid, tripropyl ester tri-n-propyl phosphate
Inchi:	InChI=1S/C9H21O4P/c1-4-7-11-14(10,12-8-5-2)13-9-6-3/h4-9H2,1-3H3
InchiKey:	RXPQRKFMDQNODS-UHFFFAOYSA-N
Formula:	C9H21O4P
SMILES:	CCCOP(=O)(OCCC)OCCC
Mol. weight [g/mol]:	224.23
CAS:	513-08-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.12		Crippen Method
logp	3.374		Crippen Method
mcvol	181.610	ml/mol	McGowan Method
rinpol	1350.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1379.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	56.70	kJ/mol	459.50	NIST Webbook
pvap	1.69e-05	kPa	263.15	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
pvap	6.03e-05	kPa	273.15	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate

pvap	2.09e-04	kPa	283.15	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
pvap	6.57e-04	kPa	293.15	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate:	https://www.doi.org/10.1021/je500428d
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C513086&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices

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