Triphenyl phosphate

Other names:	Altal
	Celluflex TPP
	Disflamoll TP
	Kronitex TPP
	NSC 57868
	Phenyl phosphate
	Phenyl phosphate ((PhO)3PO)
	Phosflex TPP
	TP
	TPP
	Trifenylfosfat
	Triphenyl phosphoric acid ester
	phosphoric acid, triphenyl ester
	triphenoxyphosphine oxide
Inchi:	InChI=1S/C18H15O4P/c19-23(20-16-10-4-1-5-11-16,21-17-12-6-2-7-13-17)22-18-14-8-3
InchiKey:	XZZNDPSIHUTMOC-UHFFFAOYSA-N
Formula:	C18H15O4P
SMILES:	O=P(Oc1ccccc1)(Oc1ccccc1)Oc1ccccc1
Mol. weight [g/mol]:	326.28
CAS:	115-86-6

Physical Properties

Property code	Value	Unit	Source
hsub	114.40 ± 2.60	kJ/mol	NIST Webbook
log10ws	-7.14		Crippen Method
logp	5.331		Crippen Method
mcvol	237.140	ml/mol	McGowan Method
rinpol	2392.00		NIST Webbook
rinpol	2320.00		NIST Webbook
rinpol	2359.00		NIST Webbook
rinpol	2330.00		NIST Webbook
rinpol	2363.00		NIST Webbook
rinpol	2366.00		NIST Webbook
rinpol	2363.00		NIST Webbook
rinpol	2363.00		NIST Webbook
rinpol	2363.00		NIST Webbook
rinpol	391.90		NIST Webbook

rinpol	391.90		NIST Webbook
ss	397.50	J/mol×K	NIST Webbook
tt	322.55 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	356.20	J/mol×K	300.00	NIST Webbook
hfust	29.61	kJ/mol	322.50	NIST Webbook
hfust	29.61	kJ/mol	322.55	NIST Webbook
hfust	29.61	kJ/mol	322.50	NIST Webbook
hvapt	81.40	kJ/mol	615.50	NIST Webbook
pvap	2.70e-07	kPa	298.00	Determination of Vapor Pressures for Organophosphate Esters
sfust	91.84	J/mol×K	322.55	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination of Vapor Pressures for Organophosphate Esters:	https://www.doi.org/10.1021/je401026a
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115866&Units=SI

Legend

cps:	Solid phase heat capacity
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
pvap:	Vapor pressure

rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tt:	Triple Point Temperature