PHOSPHINE, TRIS(2,4,6-TRIMETHOXYPHENYL)-

Inchi: InChI=1S/C27H33O9P/c1-28-16-10-19(31-4)25(20(11-16)32-5)37(26-21(33-6)12-17(29-2

InchiKey: JQKHNBQZGUKYPX-UHFFFAOYSA-N

Formula: C27H33O9P

SMILES: COc1cc(OC)c(P(c2c(OC)cc(OC)cc2OC)c2c(OC)cc(OC)cc2OC)c(OC)c1

Mol. weight [g/mol]: 532.53

Physical Properties

Property code	Value	Unit	Source
hf	-1091.31	kJ/mol	Cheméo Relay (1.0)
hvap	128.50	kJ/mol	Cheméo Relay (1.0)
ie	6.61	eV	Cheméo Relay (1.0)
log10ws	-6.62		Cheméo Relay (1.0)
logp	3.522		Crippen Method
mcvol	393.300	ml/mol	McGowan Method
tb	769.32	K	Cheméo Relay (1.0)
tf	460.88	K	Cheméo Relay (1.0)

Sources

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

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C91608150&Units=SI

Legend

hf: Enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

ie: Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point