DIETHYL 4-METHYLPHENYL PHOSPHATE

Inchi: InChI=1S/C11H17O4P/c1-4-13-16(12,14-5-2)15-11-8-6-10(3)7-9-11/h6-9H,4-5H2,1-3H3
InchiKey: UBSNERLLCAIDQQ-UHFFFAOYSA-N
Formula: C11H17O4P
SMILES: CCOP(=O)(OCC)Oc1ccc(C)cc1
Mol. weight [g/mol]: 244.23

Physical Properties

Property code	Value	Unit	Source
hvap	79.51	kJ/mol	Cheméo Relay (1.0)
ie	8.42	eV	Cheméo Relay (1.0)
log10ws	-2.18		Cheméo Relay (1.0)
logp	3.555		Crippen Method
mcvol	186.030	ml/mol	McGowan Method
rinpol	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
ripol	2310.00		NIST Webbook
ripol	2310.00		NIST Webbook
tb	573.62	K	Cheméo Relay (1.0)
tf	254.66	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4877081&Units=SI
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):

Legend

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point