

Methyldiphenyl phosphate

Other names:	Methyl diphenyl phosphate Phosphoric acid, methyl diphenyl ester
Inchi:	InChI=1S/C13H13O4P/c1-15-18(14,16-12-8-4-2-5-9-12)17-13-10-6-3-7-11-13/h2-11H,1H
InchiKey:	VOWPVJACXJNHBC-UHFFFAOYSA-N
Formula:	C13H13O4P
SMILES:	COP(=O)(Oc1ccccc1)Oc1ccccc1
Mol. weight [g/mol]:	264.22

Physical Properties

Property code	Value	Unit	Source
hf	-488.66	kJ/mol	Cheméo Relay (1.0)
hvap	91.33	kJ/mol	Cheméo Relay (1.0)
ie	8.81	eV	Cheméo Relay (1.0)
log10ws	-3.23		Cheméo Relay (1.0)
logp	3.899		Crippen Method
mcvol	190.450	ml/mol	McGowan Method
pc	2337.49	kPa	Cheméo Relay (1.0, beta)
tb	612.56	K	Cheméo Relay (1.0)
tf	310.16	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115899&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

hf:	Enthalpy of formation at standard conditions
hvac:	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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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