

Phosphoric acid, phenyl-diethyl ester

Other names:	Diethyl phenyl phosphate
Inchi:	InChI=1S/C10H15O4P/c1-3-12-15(11,13-4-2)14-10-8-6-5-7-9-10/h5-9H,3-4H2,1-2H3
InchiKey:	DHTQKXHLXVUBCF-UHFFFAOYSA-N
Formula:	C10H15O4P
SMILES:	CCOP(=O)(OCC)Oc1ccccc1
Mol. weight [g/mol]:	230.20

Physical Properties

Property code	Value	Unit	Source
af	0.5686		Cheméo Relay (1.0)
hf	-673.11	kJ/mol	Cheméo Relay (1.0)
hvap	77.04	kJ/mol	Cheméo Relay (1.0)
ie	8.86	eV	Cheméo Relay (1.0)
log10ws	-1.63		Cheméo Relay (1.0)
logp	3.247		Crippen Method
mcpvol	171.940	ml/mol	McGowan Method
pc	2241.41	kPa	Cheméo Relay (1.0, beta)
rinpol	1502.00		NIST Webbook
rinpol	1502.00		NIST Webbook
ripol	2210.00		NIST Webbook
ripol	2210.00		NIST Webbook
tb	558.66	K	Cheméo Relay (1.0)
tc	734.93	K	Cheméo Relay (1.0)
tf	249.00	K	Cheméo Relay (1.0)

Sources

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=C2510863&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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