Diazoxon

Other names:	Phosphoric acid, diethyl 6-methyl-2-(1-methylethyl)-4-pyrimidinyl ester
	Phosphoric acid, diethyl 2-isopropyl-6-methyl-4-pyrimidinyl ester
	Diazinon oxon
	Oxodiazinon
	Diazinon O-analog
Inchi:	InChI=1S/C12H21N2O4P/c1-6-16-19(15,17-7-2)18-11-8-10(5)13-12(14-11)9(3)4/h8-9H,6
InchiKey:	VBLJFQYCTRKKKF-UHFFFAOYSA-N
Formula:	C12H21N2O4P
SMILES:	CCOP(=O)(OCC)Oc1cc(C)nc(C(C)C)n1
Mol. weight [g/mol]:	288.28
CAS:	962-58-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.48		Crippen Method
logp	3.468		Crippen Method
mcvol	220.080	ml/mol	McGowan Method
rinpol	1766.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1766.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C962583&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices