

Coralox

Other names:

Phosphoric acid, 3-chloro-4-methyl-2-oxo-2H-1-benzopyran-7-yl diethyl ester
Coumarin, 3-chloro-7-hydroxy-4-methyl-, diethyl phosphate
Coroxon
Coumaphos O-analog
Coumaphos oxon
3-Chloro-4-methyl-7-coumarinyl diethyl phosphate
O,O-Di(2-chloroethyl)-7-(3-chloro-4-methylcoumarinyl)phosphate
Diethyl 3-chloro-4-methyl-7-coumarinyl phosphate
O,O-Diethyl O-(3-chloro-4-methylcoumarin-7-yl) phosphate
Phosphoric acid, diethyl ester, ester with 3-chloro-7-hydroxy-4-methylcoumarin
Co-ral-O-analog
3-chloro-4-methyl-2-oxo-2H-1-benzopyran-7-yl diethyl phosphate

Inchi:

InChI=1S/C14H16ClO6P/c1-4-18-22(17,19-5-2)21-10-6-7-11-9(3)13(15)14(16)20-12(11)

InchiKey:

FDYMERLIFOUIRZ-UHFFFAOYSA-N

Formula:

C14H16ClO6P

SMILES:

CCOP(=O)(OCC)Oc1ccc2c(C)c(Cl)c(=O)oc2c1

Mol. weight [g/mol]:

346.70

CAS:

321-54-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.41		Crippen Method
logp	4.315		Crippen Method
mcvol	232.820	ml/mol	McGowan Method

Sources

Crippen Method:

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

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C321540&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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