

# Dioxathion

## Other names:

Phosphorodithioic acid, S,S'-1,4-dioxane-2,3-diyl O,O,O',O'-tetraethyl ester

Phosphorodithioic acid, S,S'-p-dioxane-2,3-diyl O,O,O',O'-tetraethyl ester

AC 528

Delnatex

Delnav

Dioxation

ENT 22,897

Hercules 528

Kavadel

Navadel

1,4-Dioxan-2,3-Diyl bis(O,O-diethyl phosphorothiolothionate)

2,3-p-Dioxane S,S'-bis(O,O-diethyl phosphorodithioate)

2,3-p-Dioxanedithiol S,S-bis(O,O-diethyl phosphorodithioate)

2,3-Bis(diethoxyphosphinothioylthio)-1,4-dioxane

1,4-Dioxan-2,3-diyl bis(O,O-diethyl phosphorodithioate)

Bis(dithiophosphate de O,O-diethyle) de S,S'-(1,4-dioxanne-2,3-diyle)

Deltic

1,4-Diossan-2,3-diyl-bis(O,O-dietil-ditiofosfato)

2,3-P-Dioxan-S,S'-bis(O,O-diaethyl-dithiophosphat)

1,4-Dioxaan-2,3-diyl-bis(O,O-diethyl-dithiofosfaat)

1,4-Dioxan-2,3-diyl-bis(O,O-diaethyl-dithiophosphat)

Dioxane phosphate

1,4-Dioxan-2,3-diyl O,O,O',O'-tetraethyl di(phosphoromithioate)

2,3-p-Dioxandithiol S,S-bis(O,O-diethyl phosphorodithioate)

p-Dioxane-2,3-dithiol, S,S-diester with O,O-diethyl phosphorodithioate

p-Dioxane-2,3-diyl ethyl phosphorodithioate

ENT 22897

Hercules ac528

NCI-C00395

Ruphos

A mixture consisting essentially of cis- and trans-S,S'-5,5'-p-dioxane-2,3-diyl bis(O,O-diethyl phosphorodithioate)

2,3-p-Dioxane S,S'-bis(O,O-diethyl phosphorodithioate)

S,S'-1,4-Dioxane-2,3-diyl O,O,o',o'-tetraethyl bis(dithiophosphate)

Delnav I

Delnav II

## Inchi:

InChI=1S/C12H26O6P2S4/c1-5-15-19(21,16-6-2)23-11-12(14-10-9-13-11)24-20(22,17-7

## InchiKey:

VBKKVDGJXVOLNE-UHFFFAOYSA-N

## Formula:

C12H26O6P2S4

## SMILES:

CCOP(=S)(OCC)SC1OCCOC1SP(=S)(OCC)OCC

## Mol. weight [g/mol]:

456.54

CAS:

78-34-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	3.25		Crippen Method
logp	4.747		Crippen Method
mcvol	310.620	ml/mol	McGowan Method
rinpol	1775.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1751.40		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1758.00		NIST Webbook

## Sources

**Crippen Method:**<http://pubs.acs.org/doi/abs/10.1021/ci9903071>**Crippen Method:**[https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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=C78342&Units=SI>

## Legend

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

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