

Fonofos

Other names:	O-Ethyl S-phenyl ethylphosphonrothiolothionate Phosphonodithioic acid, ethyl-, O-ethyl S-phenyl ester Difonate Difonatul Dyfonat Dyfonate Dyfonate 10G Dyphonate N 2790 O-Ethyl S-Phenyl ethyldithiophosphonate O-Ethyl S-phenyl ethylphosphonodithioate Stauffer N 2790 O-Aethyl-S-phenyl-aethyl-dithiophosphonat ENT 25,796 Fonophos OMS 410 (.+/-)-O-Ethyl S-phenyl ethylphosphonodithioate
Inchi:	InChI=1S/C10H15OPS2/c1-3-11-12(13,4-2)14-10-8-6-5-7-9-10/h5-9H,3-4H2,1-2H3
InchiKey:	KVGLBTYUCJYMND-UHFFFAOYSA-N
Formula:	C10H15OPS2
SMILES:	CCOP(=S)(CC)Sc1ccccc1
Mol. weight [g/mol]:	246.33
CAS:	944-22-9

Physical Properties

Property code	Value	Unit	Source
log10ws	0.18		Crippen Method
logp	4.145		Crippen Method
mcvol	187.030	ml/mol	McGowan Method
rinpol	1779.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1754.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1773.00		NIST Webbook
rinpol	1779.00		NIST Webbook

rinp	1720.00	NIST Webbook
rip	2500.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C944229&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinp:	Non-polar retention indices
rip:	Polar retention indices

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