

Phosphorodithioic acid, S-[(tert-butylthio)methyl] O,O-diethyl ester

Other names:	AC 92.100 AC 92100 Aragran Contraven Counter Counter 15G Counter 15G soil insecticide Counter 15G soil insecticide-nematicide Cyanater ENT 27920 Methanethiol, (tert-butylthio)-, S-ester with O,O-diethyl phosphorodithioate O,O-Diethyl S-(tert-butylthio)methyl phosphorodithioate O,O-Diethyl S-[[[(1,1-dimethylethyl)thio]methyl] phosphorodithioate Phosphorodithioic acid, O,O-diethyl S-(((1,1-dimethylethyl)thio)methyl) ester Phosphorodithioic acid, S-[[[(1,1-dimethylethyl)thio]methyl] O,O-diethyl ester S-(((1,1-Dimethylethyl)thio)methyl)-O,O-diethyl phosphorodithioate S-[(tert-Butylthio)methyl] O,O-diethyl phosphorodithioate S-[[[(1,1-Dimethylethyl)thio]methyl] O,O-diethyl phosphorodithioate S-t-Butylthio-methyl-O,O-diethyl phosphorodithioate Terbufos tert-butylsulfanylmethylsulfanyl-diethoxy-sulfanylidene phosphorane
Inchi:	InChI=1S/C9H21O2PS3/c1-6-10-12(13,11-7-2)15-8-14-9(3,4)5/h6-8H2,1-5H3
InchiKey:	XLNZEKHULJKQBA-UHFFFAOYSA-N
Formula:	C9H21O2PS3
SMILES:	CCOP(=S)(OCC)SCSC(C)(C)C
Mol. weight [g/mol]:	288.43
CAS:	13071-79-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.46		Aqueous Solubility Prediction Method
log10ws	-4.75		Estimated Solubility Method
logp	4.506		Crippen Method
mcvol	218.920	ml/mol	McGowan Method
rinpol	1781.00		NIST Webbook

rinpol	1748.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1777.00		NIST Webbook
rinpol	1783.00		NIST Webbook
tf	243.95	K	Aqueous Solubility Prediction Method

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13071799&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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