

Trichloronat

Other names:	5082A
	Agrisil
	Agritox
	BAY 37289
	Bayer 37289
	Bayer 5081
	Bayer S 4400
	Chemagro 37289
	ENT 25,712
	ENT-25712
	Ethyl trichlorophenylethylphosphonothioate
	Fenophosphon
	Fitosol
	O-Aethyl-O-(2,4,5-trichlorphenyl)-aethylthionophosponat
	O-Ethyl O-2,4,5-Trichlorophenyl ethylphosphonothioate
	OMS 412
	OMS 578
	Phenol, 2,4,5-trichloro-, O-ester with O-ethyl ethylphosphonothioate
	Phosphonothioic acid, ethyl-, O-ethyl O-(2,4,5-trichlorophenyl) ester
	Phytosol
	Richloronate
	S 4400
	Stauffer N-3049
	Trichloronate
	Wirkstoff 37289
	ethoxy-ethyl-sulfanylidene-(2,4,5-trichlorophenoxy)phosphorane
Inchi:	InChI=1S/C10H12Cl3O2PS/c1-3-14-16(17,4-2)15-10-6-8(12)7(11)5-9(10)13/h5-6H,3-4H2
InchiKey:	ANIAQSUBRGXWLS-UHFFFAOYSA-N
Formula:	C10H12Cl3O2PS
SMILES:	CCOP(=S)(CC)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	333.60
CAS:	327-98-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.75		Aqueous Solubility Prediction Method

log10ws	-5.75		Estimated Solubility Method
logp	5.392		Crippen Method
mcvol	213.270	ml/mol	McGowan Method

Sources

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

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=C327980&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

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

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