

Etridiazole

Other names:	1,2,4-Thiadiazole, 5-ethoxy-3-(trichloromethyl)- Terrazole Aaterra Echlomezol Echlomezole Ethazol Ethazole (fungicide) ETMT Koban Olin Mathieson 2,424 OM 2424 Terracoat L21 Truban Banrot Etcmtb Ethazole Etridiazol OM 2425 Terrachlor-super X Terracoat 3-(Trichloromethyl)-5-ethoxy-1,2,4-thiadiazole 5-Aethoxy-3-trichlormethyl-1,2,4-thiadiazol 5-Ethoxy-3-(trichloromethyl)-1,2,4-thiadiazole Dwell MF-344 Pansoil Terraflo 5-Ethoxy-3-trichloromethyl-1,2,4-thiadiazol Etridazole NSC 524929 Planvate
Inchi:	InChI=1S/C5H5Cl3N2OS/c1-2-11-4-9-3(10-12-4)5(6,7)8/h2H2,1H3
InchiKey:	KQTVWCSONPJPE-UHFFFAOYSA-N
Formula:	C5H5Cl3N2OS
SMILES:	CCOc1nc(C(Cl)(Cl)Cl)ns1
Mol. weight [g/mol]:	247.53
CAS:	2593-15-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.30		Crippen Method
logp	2.764		Crippen Method
mcvol	140.750	ml/mol	McGowan Method
rinpol	1452.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1452.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1409.00		NIST Webbook
ripol	2004.00		NIST Webbook
ripol	2004.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2593159&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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