

Etaconazole

Other names:	1H-1,2,4-Triazole, 1-[[2-(2,4-dichlorophenyl)-4-ethyl-1,3-dioxolan-2-yl]methyl]- ETACONAZOLE-«alpha» (ESO) ETACONAZOLE-«beta» (ESO) 1-[[2-(2,4-dichlorophenyl)-4-ethyl-1,3-dioxolan-2-yl]methyl]-1H-1,2,4-triazole
Inchi:	InChI=1S/C14H15Cl2N3O2/c1-2-11-6-20-14(21-11,7-19-9-17-8-18-19)12-4-3-10(15)5-13
InchiKey:	DWRKFAJEBUWTQM-UHFFFAOYSA-N
Formula:	C14H15Cl2N3O2
SMILES:	CCC1COC(Cn2cncn2)(c2ccc(Cl)cc2Cl)O1
Mol. weight [g/mol]:	328.19
CAS:	60207-93-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	3.263		Crippen Method
mcvol	220.200	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60207934&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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