

1H-1,2,4-Triazole, 1-[2-(2,4-dichlorophenyl)-3-(1,1,2,2-tetrafluoroethoxy)propyl]-

Other names: 1-[2-(2,4-Dichlorophenyl)-3-(1,1,2,2-tetrafluoroethoxy)propyl]-1,2,4-triazole; TETRACONAZOLE; Tetraconazol.

InChI: InChI=1S/C13H11Cl2F4N3O/c14-9-1-2-10(11(15)3-9)8(4-22-7-20-6-21-22)5-23-13(18,19)12(16)17/h1-3,6-8,12H,4-5H2

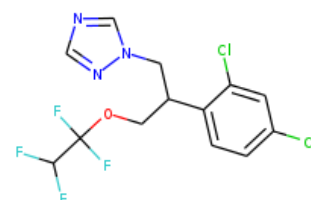
InChI Key: LQDARGUHUSPFNL-UHFFFAOYSA-N

Formula: C13H11Cl2F4N3O

SMILES: FC(F)C(F)(F)OCC(Cn1cncn1)c1ccc(Cl)cc1Cl

Molecular Weight: 372.15

CAS: 112281-77-3



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	4.24		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C13H11Cl2F4N3O/c14-9-1-2-10\(11\(15\)3-9\)8\(4-22-7-20-6-21-22\)5-23-13\(18,19\)12\(16\)17/h1-3,6-8,12H,4-5H2](http://webbook.nist.gov/cgi/inchi/InChI=1S/C13H11Cl2F4N3O/c14-9-1-2-10(11(15)3-9)8(4-22-7-20-6-21-22)5-23-13(18,19)12(16)17/h1-3,6-8,12H,4-5H2)

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

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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