

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

Other names:

TETRACONAZOLE

1-[2-(2,4-Dichlorophenyl)-3-(1,1,2,2-tetrafluoroethoxy)propyl]-1,2,4-triazole

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)

InchiKey: LQDARGUHUSPFNL-UHFFFAOYSA-N

Formula: C13H11Cl2F4N3O

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

Mol. weight [g/mol]: 372.15

CAS: 112281-77-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.68		Crippen Method
logp	4.243		Crippen Method
mcvol	218.180	ml/mol	McGowan Method
rinpol	2013.00		NIST Webbook
rinpol	1998.00		NIST Webbook

Sources

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>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C112281773&Units=SI>

Legend

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

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