

Fluotrimazole

Other names:

1-[di(phenyl)-[3-(trifluoromethyl)phenyl]methyl]-1,2,4-triazole
1-[diphenyl[3-(trifluoromethyl)phenyl]methyl]-1H-1,2,4-triazole
1H-1,2,4-Triazole, 1-[diphenyl[3-(trifluoromethyl)phenyl]methyl]-
B 6660
Fluotrimazol
NSC 303302
Persulon
Persulon 6660

Inchi:

InChI=1S/C22H16F3N3/c23-22(24,25)20-13-7-12-19(14-20)21(28-16-26-15-27-28,17-8-3

InchiKey:

LXMQMMSGERCRSU-UHFFFAOYSA-N

Formula:

C22H16F3N3

SMILES:

FC(F)(F)c1cccc(C(c2ccccc2)(c2ccccc2)n2cncn2)c1

Mol. weight [g/mol]:

379.38

CAS:

31251-03-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.40		Aqueous Solubility Prediction Method
logp	5.137		Crippen Method
mcvol	265.350	ml/mol	McGowan Method

Sources

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

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C31251033&Units=SI>

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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<https://www.cheméo.com/cid/72-468-3/Fluotrimazole.pdf>

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