

Flutriafol

Other names:

(±)-a-(2-fluorophenyl)-a-(4-fluorophenyl)-1H-1,2,4-triazole-1-ethanol
($\hat{\pm}$)-a-(2-fluorophenyl)-a-(4-fluorophenyl)-1H-1,2,4-triazole-1-ethanol
.alpha.-(2-fluorophenyl)-.alpha.-(4-fluorophenyl)-1H-1,2,4-triazole-1-ethanol
1-(2-fluorophenyl)-1-(4-fluorophenyl)-2-(1,2,4-triazol-1-yl)ethanol
1H-1,2,4-Triazole-1-ethanol, «alpha»-(2-fluorophenyl)-«alpha»-(4-fluorophenyl)-
1H-1,2,4-Triazole-1-ethanol,
Â«alphaÂ»-(2-fluorophenyl)-Â«alphaÂ»-(4-fluorophenyl)-
Impact

PP 450

R 152450

«alpha»-(2-Fluorophenyl)-«alpha»-(4-fluorophenyl)-1H-1,2,4-triazole-1-ethanol

Â«alphaÂ»-(2-Fluorophenyl)-Â«alphaÂ»-(4-fluorophenyl)-1H-1,2,4-triazole-1-ethanol

Inchi: InChI=1S/C16H13F2N3O/c17-13-7-5-12(6-8-13)16(22,9-21-11-19-10-20-21)14-3-1-2-4-1

InchiKey: JWUCHKBSVLQQCO-UHFFFAOYSA-N

Formula: C16H13F2N3O

SMILES: OC(Cn1cncn1)(c1ccc(F)cc1)c1ccccc1F

Mol. weight [g/mol]: 301.29

CAS: 76674-21-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.37		Aqueous Solubility Prediction Method
log10ws	-3.37		Estimated Solubility Method
logp	2.492		Crippen Method
mcvol	208.670	ml/mol	McGowan Method
rinpol	2152.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2157.00		NIST Webbook

Sources

Measurement and Correlation of the Solubilities of Azoxystrobin, Flutriafol, and its Concomitant in Subcritical 1,1,1,2-Tetrafluoroethane:
Aqueous Solubility Prediction Method:
Estimated Solubility Method:

<https://www.doi.org/10.1021/acs.jced.8b00240>

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C76674210&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/29-749-9/Flutriafol.pdf>

Generated by Cheméo on 2024-04-19 16:45:49.585031486 +0000 UTC m=+15834398.505608805.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.