

Fludioxonil

Other names:

1H-Pyrrole-3-carbonitrile, 4-(2,2-difluoro-1,3-benzodioxol-4-yl)-
4-(2,2-Difluoro-1,3-benzodioxol-4-yl)-1H-pyrrole-3-carbonitrile
Celeste
Fludioxinil
Geoxe
Savior

Inchi:

InChI=1S/C12H6F2N2O2/c13-12(14)17-10-3-1-2-8(11(10)18-12)9-6-16-5-7(9)4-15/h1-3,4

InchiKey:

MUJOIMFVNIBMKC-UHFFFAOYSA-N

Formula:

C12H6F2N2O2

SMILES:

N#Cc1c[nH]cc1-c1cccc2c1OC(F)(F)O2

Mol. weight [g/mol]:

248.19

CAS:

131341-86-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.21		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	2.393		Crippen Method
mvol	152.500	ml/mol	McGowan Method
rinpol	2169.00		NIST Webbook
rinpol	2169.00		NIST Webbook

Sources

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C131341861&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Aqueous and cosolvent solubility data for drug-like organic compounds:

<https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/>

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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<https://www.chemeo.com/cid/33-660-2/Fludioxonil.pdf>

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