

Fluthiacet-methyl

Other names: Acetic acid,
Inchi: 2-[[2-chloro-4-fluoro-5-[(tetrahydro-3-oxo-1H-3H-[1,3,4]thiadiazolo[3,4-a]pyridazin-1-ylidene)methyl]ester
InchiKey: ZCNQYNHDVRPZIH-UHFFFAOYSA-N
Formula: C15H15ClFN3O3S2
SMILES: COC(=O)CSc1cc(N=c2sc(=O)n3n2CCCC3)c(F)cc1Cl
Mol. weight [g/mol]: 403.88
CAS: 117337-19-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	2.795		Crippen Method
mcvol	258.090	ml/mol	McGowan Method
rinpol	3244.00		NIST Webbook
rinpol	3244.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C117337196&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/61-352-3/Fluthiacet-methyl.pdf>

Generated by Cheméo on 2024-05-01 07:20:00.527665487 +0000 UTC m=+16837249.448242802.

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