ISOXAFLUTOLE

Other names:	(5-Cyclopropylisoxazol-4-yl)-[2-methylsulfonyl-4-(trifluoromethyl)phenyl]methanone Methanone, (5-cyclopropyl-4-isoxazolyl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl]- (5-cyclopropyl-4-isoxazolyl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl]methanone
Inchi:	InChI=1S/C15H12F3NO4S/c1-24(21,22)12-6-9(15(16,17)18)4-5-10(12)13(20)11-7-19-23
InchiKey:	OYIKARCXOQLFHF-UHFFFAOYSA-N
Formula:	C15H12F3NO4S
SMILES:	CS(=O)(=O)c1cc(C(F)(F)F)ccc1C(=O)c1cnoc1C1CC1
Mol. weight [g/mol]:	359.32
CAS:	141112-29-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.81		Crippen Method
logp	3.205		Crippen Method
mcvol	218.950	ml/mol	McGowan Method
rinpol	2283.00		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=C141112290&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