

Flumazenil

Other names:

4H-Imidazo(1,5-a)(1,4)benzodiazepine-3-carboxylic acid,
8-fluoro-5,6-dihydro-5-methyl-6-oxo-, ethyl ester
Anexate

Flumazepil

Ro-15-1788

Ethyl

8-fluoro-5,6-dihydro-5-methyl-6-oxo-4H-imidazo[1,5-a][1,4]benzodiazepine-3-carboxylate

Ethyl

8-fluoro-5,6-dihydro-5-methyl-6-oxo-4H-imidazo[1,5-a][1,4]benzodiazepin-3-carboxylate

Lanexat

Mazicon

Ro-15-1788/000

Romazicon

Ro 151788

flumazenil (Ro-15-1788)

Inchi: InChI=1S/C15H14FN3O3/c1-3-22-15(21)13-12-7-18(2)14(20)10-6-9(16)4-5-11(10)19(12)

InchiKey: OFBIFZUFASYRE-UHFFFAOYSA-N

Formula: C15H14FN3O3

SMILES: CCOC(=O)c1ncn2c1CN(C)C(=O)c1cc(F)ccc1-2

Mol. weight [g/mol]: 303.29

CAS: 78755-81-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Crippen Method
logp	1.774		Crippen Method
mcvol	208.850	ml/mol	McGowan Method
rinpola	2560.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C78755814&Units=SI>

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>

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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