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DATASHEET

Escitalopram oxalate

Product overview

Name	Escitalopram oxalate
Cat No	HB1804
Biological action	Inhibitor
Purity	>99%
Description	Selective serotonin reuptake inhibitor (SSRI)

Biological Data

Biological description	Selective serotonin reuptake inhibitor (SSRI) (K_i values are 0.89, 8150, and 10500 nM for SET, NET and DAT transporters respectively).
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Solubility & Handling

Storage instructions	+4 °C
Solubility overview	Soluble in water (50mM) and in DMSO (100mM)
Important	This product is for RESEARCH USE ONLY and is not intended for therapeutic or diagnostic use. Not for human or veterinary use.

Chemical Data

Chemical name	(+)-(S)-1-[3-(Dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofurancar bonitrile oxalate
Molecular Weight	414.43
Molecular Formula	$C_{20}H_{21}FN_2O \cdot C_2H_2O_4$
CAS Number	219861-08-2
PubChem identifier	146571
SMILES	<chem>CN(C)CCC[C@@]1(C2=C(CO1)C=C(C=C2)C#N)C3=CC=C(C=C3)F.C(=O)(C(=O)O)O</chem>
InChi	InChI=1S/C20H21FN2O.C2H2O4/c1-23(2)11-3-10-20(17-5-7-18(21)8-6-17)19-9-4-15(13-22)12-16(19)14-24-20;3-1(4)2(5)6/h4-9,12H,3,10-11,14H2,1-2H3;(H,3,4)(H,5,6)/t20-/m0./s1
InChiKey	KTGRHKOEFSJQNS-BDQAORGHSA-N
MDL number	MFCD06407826