Furethidine

Other names:	4-Piperidinecarboxylic acid, 4-phenyl-1-[2-[(tetrahydro-2-furanyl)methoxy]ethyl]-, ethyl ester
	Isonipecotic acid, 4-phenyl-1-[2-[(tetrahydrofurfuryl)oxy]ethyl]-, ethyl ester
	Ethyl 4-phenyl-1-[2-[(tetrahydrofurfuryl)oxy]ethyl]isonipecotate
	Ethyl 4-phenyl-1-(2-tetrahydrofurfuryloxyethyl)piperidine-4-carboxylate
	1-(2-Tetrahydrofurfuryloxyethyl)-4-phenylpiperidine-4-carboxylic acid ethyl ester
Inchi:	InChI=1S/C21H31NO4/c1-2-25-20(23)21(18-7-4-3-5-8-18)10-12-22(13-11-21)14-16-24-1
InchiKey:	NNCOZXNZFLUYGG-UHFFFAOYSA-N
Formula:	C21H31NO4
SMILES:	CCOC(=O)C1(c2ccccc2)CCN(CCOCC2CCCO2)CC1
Mol. weight [g/mol]:	361.48
CAS:	2385-81-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.90		Crippen Method
logp	2.779		Crippen Method
mcvol	290.430	ml/mol	McGowan Method
rinpol	2637.00		NIST Webbook

Sources

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=C2385811&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

rinpol: Non-polar retention indices