Sulpiride

Other names:	(+) N-1-(ethylpyrrolidin-2-ylmethyl)-2-methoxy-5-sulfamoylbenzamide (sulpiride) (.+/-.)-Sulpiride 5-(Aminosulfonyl)-N-((1-ethyl-2-pyrrolidinyl)methyl)-2-methoxybenzamide Abilit Aiglonyl Benzamide, 5-(aminosulfonyl)-N-[(1-ethyl-2-pyrrolidinyl)methyl]-2-methoxy- Coolspan Dobren Dogmatil Dogmatyl Dolmatil Eglonyl Guastil Meresa Miradol Mirbanil Misulvan N-((1-Ethyl-2-pyrrolidinyl)methyl)-2-methoxy-5-sulfamoylbenzamide N-((1-Ethyl-2-pyrrolidinyl)methyl)-5-sulfamoyl-o-anisamide Neogama Omperan Pyrikappl Pyrkappl R.D. 1403 RD 1403 Sernevin Splotin Sulpirid Sulpitil Sulpyrid Sursumid Synedil Trilan dl-Sulpiride o-Anisamide, N-((1-ethyl-2-pyrrolidinyl)methyl)-5-sulfamoyl-
Inchi:	InChI=1S/C15H23N3O4S/c1-3-18-8-4-5-11(18)10-17-15(19)13-9-12(23(16,20)21)6-7-14(
InchiKey:	BGRJTUBHPOOWDU-UHFFFAOYSA-N
Formula:	C15H23N3O4S
SMILES:	CCN1CCCC1CNC(=O)c1cc(S(N)(=O)=O)ccc1OC
Mol. weight [g/mol]:	341.43

CAS: 15676-16-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Aqueous Solubility Prediction Method
logp	0.557		Crippen Method
mcvol	253.060	ml/mol	McGowan Method
rinpol	3074.00		NIST Webbook
rinpol	3074.00		NIST Webbook
tf	451.48	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	46.15	kJ/mol	451.00	NIST Webbook

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15676161&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hfust: Enthalpy of fusion at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

tf: Normal melting (fusion) point