SULPHAPHENAZOLE

Other names:	1-Phenyl-5-sulfanilamidopyrazole
	3-(p-Aminobenzenesulfonamido)-2-phenylpyrazole
	4-Amino-N-(1-phenyl-1H-pyrazol-5-yl)benzenesulfonamide
	5-Sulfanilamido-1-phenylpyrazole
	Benzenesulfonamide, 4-amino-N-(1-phenyl-1H-pyrazol-5-yl)-
	Depocid
	Depotsulfonamide
	Eftolon
	Firmazolo
	Inamil
	Isarol
	Isarol V
	Merian
	Microtan pirazolo
	N'-(1-Phenylpyrazol-5-yl)sulfanilamide
	N1-(1-Phenylpyrazol-5-yl)sulfanilamide
	Orisul
	Orisulf
	Paidazolo
	Plisulfan
	Pyrazole, 1-phenyl-5-sulfanilamido-
	Raziosulfa
	Sulfabid
	Sulfafenazolo
	Sulfanilamide, N1-(1-phenylpyrazol-5-yl)-
	Sulfaphenazol
	Sulfaphenazon
	Sulfaphenylpipazol
	Sulfaphenylpyrazole
	Sulphenazole
	sulfaphenazole
Inchi:	InChI=1S/C15H14N4O2S/c16-12-6-8-14(9-7-12)22(20,21)18-15-10-11-17-19(15)13-4-2-1
InchiKey:	QWCJHSGMANYXCW-UHFFFAOYSA-N
Formula:	C15H14N4O2S
SMILES:	Nc1ccc(S(=O)(=O)Nc2ccnn2-c2ccccc2)cc1
Mol. weight [g/mol]:	314.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.32		Aqueous Solubility Prediction Method
logp	2.255		Crippen Method
mcvol	223.240	ml/mol	McGowan Method
tf	460.86	K	Cheméo Relay (1.0)

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C526089&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point