

Sulfaphenazole

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
Sulphaphenazole
Sulphenazole

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-

InchiKey:

QWCJHSGMANYXCW-UHFFFAOYSA-N

Formula:

C15H14N4O2S

SMILES:

Nc1ccc(S(=O)(=O)Nc2ccnn2-c2ccccc2)cc1

Mol. weight [g/mol]:

314.36

CAS:

526-08-9

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

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C526089&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

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

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