Sulfapyridine

Other names:

2-(p-Aminobenzenesulphonamido)pyridine
2-Sulfanilamidopyridin
2-Sulfanilamidopyridine
2-Sulfanilylaminopyridine
2-Sulfapyridine
4-Amino-N,2-pyridinylbenzenesulfonamide
4-Amino-N-2-pyridinylbenzenesulfonamide (sulfapyridine)
4-[(2-Pyridylamino)sulfonyl]aniline
4-amino-N-2-pyridinylbenzenesulfonamide
4-amino-N-pyridin-2-ylbenzenesulfonamide
A-499
Adiplon
Benzenesulfonamide, 4-amino-N-2-pyridinyl-
Coccoclase
Dagenan
Eubasin
Eubasinum
Haptocil
M and B 693
M&B-693
M+B 693
N-2-Pyridylsulfanilamide
N-2-pyridinylsulfanilamide
N1-2-Pyridylsulfanilamide
NSC 41791
NSC 4753
Piridazol
Plurazol
Pyriamid
Pyridazol
Relbapiridina
Ronin
Septipulmon
Streptosilpyridine
Sulfanilamide, N1-2(1H)-pyridylidene-
Sulfanilamide, N1-2-pyridyl-
Sulfidin
Sulfidine
Sulphapyridine
Thioseptal

	Trianon
Inchi:	InChI=1S/C11H11N3O2S/c12-9-4-6-10(7-5-9)17(15,16)14-11-3-1-2-8-13-11/h1-8H,12H2
InchiKey:	GECHUMIMRBOMGK-UHFFFAOYSA-N
Formula:	C11H11N3O2S
SMILES:	Nc1ccc(S(=O)(=O)Nc2ccccn2)cc1
Mol. weight [g/mol]:	249.29
CAS:	144-83-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.83		Aqueous Solubility Prediction Method
logp	1.465		Crippen Method
mcvol	176.360	ml/mol	McGowan Method
tf	464.98	K	Aqueous Solubility Prediction Method
tf	466.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	40.47	kJ/mol	462.70	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=C144832&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of sulfapyridine in propylene glycol + water mixtures and correlation with the Jouyban Acree model:	https://www.doi.org/10.1016/j.fluid.2012.12.017

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
tf:	Normal melting (fusion) point