Sulfisoxazole

Other names:

3,4-Dimethyl-5-sulfanilamidoisoxazole
3,4-Dimethyl-5-sulfonamidoisoxazole
3,4-Dimethylisoxazole-5-sulfanilamide
3,4-Dimethylisoxazole-5-sulphanilamide
4-Amino-N-(3,4-dimethyl-5-isoxazolyl)benzenesulphonamide
4-amino-N-(3,4-dimethyl-1,2-oxazol-5-yl)benzenesulfonamide
5-(4-Aminophenylsulfonamido)-3,4-dimethylisoxazole
5-(4-Aminophenylsulphonamido)-3,4-dimethylisoxazole
5-(p-Aminobenzenesulfonamido)-3,4-dimethylisooxale
5-(p-Aminobenzenesulfonamido)-3,4-dimethylisoxazole
5-(p-Aminobenzenesulphonamide)-3,4-dimethylisoxazole
5-(p-Aminobenzenesulphonamido)-3,4-dimethylisoxazole
5-Sulfanilamido-3,4-dimethylisoxazole
Accuzole
Alphazole
Amidoxal
Astrazolo
Azo gantrisin
Azosulfizin
Bactesulf
Barazae
Benzenesulfonamide, 4-amino-N-(3,4-dimethyl-5-isoxazolyl)-
Chemouag
Cosoxazole
Dorsulfan Warthausen
Entusil
Entusul
G-sox
Gantrisin
Gantrisona
Gantrosan
Isoxamin
N
N'-(3,4)Dimethylisoxazol-5-yl-sulphanilamide
N(Sup1)-(3,4-Dimethyl-5-isoxazolyl)sulfanilamide
NCI-C50022
Neazolin
Neoxazol
Norilgan-S
Pancid

Renosulfan
Roxosul tablets
SK-Soxazole
Sosol
Soxisol
Soxo
Soxomide
Stansin
Sulbio
Sulfadimethylisoxazole
Sulfafurazol
Sulfafurazole
Sulfagan
Sulfaisoxazole
Sulfalar
Sulfanilamide, N(sup1)-(3,4-dimethyl-5-isoxazolyl)-
Sulfanilamide, N.sup1.-(3,4-dimethyl-5-isoxazolyl)-
Sulfasol
Sulfasoxazole
Sulfazin
Sulfisonazole
Sulfisoxasole
Sulfisoxazol
Sulfisoxazole dialamine
Sulfizin
Sulfofurazole
Sulfoxol
Sulphafurazole
Sulsoxin
Thiasin
Unisulf
Uritrisin
V-Sul

Inchi: InChI=1S/C11H13N3O3S/c1-7-8(2)13-17-11(7)14-18(15,16)10-5-3-9(12)4-6-10/h3-6,14H

InchiKey: NHUHCSRWZMLRLA-UHFFFAOYSA-N

Formula: C11H13N3O3S

SMILES: Cc1noc(NS(=O)(=O)c2ccc(N)cc2)c1C

Mol. weight [g/mol]: 267.30

CAS: 127-69-5

Physical Properties

Property code	Value	Unit	Source
chs	-5036.40 ± 3.80	kJ/mol	NIST Webbook
hfs	-180.10 ± 3.80	kJ/mol	NIST Webbook
log10ws	-2.15		Aqueous Solubility Prediction Method
logp	1.674		Crippen Method
mcvol	186.530	ml/mol	McGowan Method
tf	466.45	K	Aqueous Solubility Prediction Method
tf	468.20 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	8.41	kJ/mol	448.20	NIST Webbook

Sources

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

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=C127695&Units=SI

Legend

chs: Standard solid enthalpy of combustion

hfs: Solid phase enthalpy of formation at standard conditions

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