

Sulfadiazine

Other names:	2-(4-Aminobenzenesulfonamido)pyrimidine
	2-(4-Aminobenzenesulfonylamino)pyrimidine
	2-(p-Aminobenzenesulfonamido)pyrimidin
	2-Sulfanilamidopyrimidine
	2-Sulfanilylaminopyrimidine
	2-Sulfapyrimidine
	4-Amino-N-(2-pyrimidinyl)benzene sulfonamide (sulfadiazine)
	4-[[[(Pyrimidin-2-yl)amino]sulfonyl]aniline
	4-amino-N-2-pyrimidinylbenzenesulfonamide
	A-306
	Adiazin
	Adiazine
	Benzenesulfonamide, 4-amino-N-2-pyrimidinyl-
	Coco-Diazine
	Codiazine
	Cremodiazine
	Cremotres
	Debenal
	Deltazina
	Di-Azo-Mul
	Diazin
	Diazolone
	Diazovit
	Diazyl
	Eskadiazine
	Honey diazine
	Lipo-Diazine
	Lipo-Levazine
	Liquadiazine
	Metha-Meridiazine
	Microsulfon
	N(Sup1)-2-Pyrimidinylsulfanilamide
	N(Sup1)-2-Pyrimidylsulfanilamide
	N1-2-Pyrimidinylsulfanilamide
	N1-2-Pyrimidylsulfanilamide
	Neazine
	Neotrizine
	Palatrize
	Pecta-diazine, suspension
	Piridisir

Pirimal
Pyrimal
Pyrimidine, 2-sulfanilamido-
Quadetts
Quadramoid
RP 2616
S. N. 112
SDA
Sanodiazine
Silvadene
Spofadrizine
Sterazine
Sulfadiazene
Sulfadiazin
Sulfadiazina Reig Jofre
Sulfanilamide, N1-2(1H)-pyrimidinylidene-
Sulfanilamide, N1-2-pyrimidinyl-
Sulfanilamidopyrimidine
Sulfapirimidin
Sulfapyrimidin
Sulfapyrimidine
Sulfatryl
Sulfazin
Sulfazine
Sulfolex
Sulfonsol
Sulfose
Sulphadiazine
Sulphadiazine E
Terfonyl
Theradiazine
Thi-Di-Mer
Tri-Sulfameth
Trifonamide
Triple Sulfas
Trisem
Truozine

Inchi:

InChI=1S/C10H10N4O2S/c11-8-2-4-9(5-3-8)17(15,16)14-10-12-6-1-7-13-10/h1-7H,11H2

InchiKey:

SEEPANYCNGTZFQ-UHFFFAOYSA-N

Formula:

C10H10N4O2S

SMILES:

Nc1ccc(S(=O)(=O)Nc2ncccn2)cc1

Mol. weight [g/mol]:

250.28

CAS:

68-35-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Aqueous Solubility Prediction Method
logp	0.860		Crippen Method
mcvol	172.250	ml/mol	McGowan Method
rinpol	2523.00		NIST Webbook
tf	527.27	K	Aqueous Solubility Prediction Method
tf	538.80 ± 0.50	K	NIST Webbook
tf	534.00 ± 3.00	K	NIST Webbook
tf	531.00 ± 4.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	44.30	kJ/mol	532.70	NIST Webbook
hfust	44.30	kJ/mol	520.40	NIST Webbook
hfust	31.20	kJ/mol	538.70	NIST Webbook
hfust	31.20	kJ/mol	538.70	NIST Webbook

Sources

Crippen Method:

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

Solubility and preferential solvation of sulfadiazine in methanol + water mixtures at several temperatures and preferential solvation of sulfadiazine in 50:50 mixture of Sulfadiazine solvent Sulfamethazine, Sulfadimethoxine, Sulfamethins of Sulfadiazine in Methanol, Ethanol, 1-Propanol, 2-Propanol, Acetone and Diethyl Ether from Method: Sulfamethoxazole and Sulfadiazine (29.15 to 31.15) Kyrzazine in Water from McGowan Method (29.15 to 33.15) K:

<https://www.doi.org/10.1016/j.fluid.2014.07.013>

<https://www.doi.org/10.1016/j.fluid.2015.03.046>

<https://www.doi.org/10.1021/je0603978>

<https://www.doi.org/10.1021/je900742p>

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C68359&Units=SI>

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
rinpola:	Non-polar retention indices
tf:	Normal melting (fusion) point

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