Benzenesulfonamide, 4-amino-N-2-thiazolyl-

Other names:

2-(Sulfanilylamino)thiazole
2-(p-Aminobenzenesulfonamido)thiazole
2-(p-Aminobenzenesulphonamido)thiazole
2-Sulfanilamidothiazol
2-Sulfanilamidothiazole
2-Sulfathiazole
2090 R.P.
4-Amino-N-2-thiazolylbenzenesulfonamide
4-Amino-N-2-thiazolylbenzenesulfonamide (sulfathiazole)
4-[(1,3-Thiazol-2-yl)aminosulfonyl]aniline
Azoquimiol
Azoseptale
Cerazol
Cerazol (suspension)
Cerazole
Chemosept
Ciba 3714
Cibazol
Coco-Thiazole
Duatok
Dulana
Eleudron
Enterobiocine
Estafilol
Formosulfathiazole
M&B 760
M+B 760
N'-(2-Thiazolyl)sulfanilamide
N(Sup1)-(2-Thiazolyl)sulfanilamide
N-(2-thiazolyl)sulfanilamide
N-1-2-Thiazolylsulfanilamide
Neostrepsan
Norsulfasol
Norsulfazole
Planomide
Poliseptil
RP 2090
Sanotiazol
Septozol
Streptosilthiazole

Sulfamul
Sulfanilamide, N(sup1)-2-thiazolyl-
Sulfanilamide, N1-2-thiazolyl-
Sulfanilamide, N1-4-thiazolin-2-ylidene-
Sulfanilamidothiazole
Sulfathiazol
Sulfavitina
Sulfocerol
Sulphathiazole
Sulzol
Thiacoccine
Thiasulfol
Thiazamide
Thiozamide
USAF SN-9
Wintrazole
sulfathiazole

Inchi: InChI=1S/C9H9N3O2S2/c10-7-1-3-8(4-2-7)16(13,14)12-9-11-5-6-15-9/h1-6H,10H2,(H,11

InchiKey: JNMRHUJNCSQMMB-UHFFFAOYSA-N

Formula: C9H9N3O2S2

SMILES: Nc1ccc(S(=O)(=O)Nc2nccs2)cc1

Mol. weight [g/mol]: 255.32

Physical Properties

Property code	Value	Unit	Source
hvap	115.58	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.37		Aqueous Solubility Prediction Method
logp	1.526		Crippen Method
mcvol	168.830	ml/mol	McGowan Method
tf	475.25	K	Aqueous Solubility Prediction Method
tf	473.40 ± 1.00	K	NIST Webbook
tf	437.00 ± 0.50	K	NIST Webbook
tf	474.70 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	30.30	kJ/mol	473.00	NIST Webbook

Sources

Effect of presence of alpha-cyclodextrin and beta-cyclodextrin on solution behavior of sulfathiazole at different temperatures. Thermodynamic and spectroscopic studies:	https://www.doi.org/10.1016/j.jct.2017.12.017
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72140&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

hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point