Sulfanilamide

Other names:

(4-(Aminosulfonyl)phenyl)amine
1162 F
4-(Aminosulfonyl)aniline
4-Aminobenzenesulfonamide
4-Aminophenylsulfonamide
4-Sulfamoylaniline
A-349
Albexan
Albosal
Ambeside
Aniline-p-sulfonic amide
Astreptine
Astrocid
Bacteramid
Bactesid
Benzenesulfonamide, 4-amino-
Benzenesulfonamide, p-amino-
Collomide
Colsulanyde
Copticide
Deseptyl
Dipron
Ergaseptine
Erysipan
Estreptocida
Exoseptoplix
F 1162
Fourneau 1162
Gerison
Gombardol
Infepan
Lusil
Lysococcine
Neococcyl
Orgaseptine
PABS
Prontalbin
Prontosil I
Prontosil album
Prontosil white

Prontylin
Pronzin album
Proseptal
Proseptine
Proseptol
Pysococcine
Rubiazol A
Sanamid
Septamide album
Septanilam
Septinal
Septolix
Septoplex
Septoplix
Stopton album
Stramid
Strepamide
Strepsan
Streptagol
Streptamid
Streptamin
Streptasol
Streptocid
Streptocid album
Streptocide
Streptocide white
Streptoclase
Streptocom
Streptol
Strepton
Streptopan
Streptosil
Streptozol
Streptozone
Streptrocide
Sulfamidyl
Sulfamine
Sulfana
Sulfanalone
Sulfanidyl
Sulfanil
Sulfanilamide Vaginal Cream
Sulfanilimidic acid

Sulfocidin
Sulfocidine
Sulfonamide
Sulfonamide P
Sulfonylamide
Sulphanilamide
Sulphonamide
Therapol
Tolder
White streptocide
antiStrept
p-Aminobenzenesulfamide
p-Aminobenzenesulfonamide
p-Aminobenzenesulfonylamide
p-Aminobenzensulfonamide
p-Aminophenylsulfonamide
p-Anilinesulfonamide
p-Sulfamidoaniline
p-Sulfamoylaniline

Inchi: InChI=1S/C6H8N2O2S/c7-5-1-3-6(4-2-5)11(8,9)10/h1-4H,7H2,(H2,8,9,10)

InchiKey: FDDDEECHVMSUSB-UHFFFAOYSA-N

Formula: C6H8N2O2S

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

Mol. weight [g/mol]: 172.21

CAS: 63-74-1

Physical Properties

Property code	Value	Unit	Source
chs	-2788.50 ± 1.60	kJ/mol	NIST Webbook
chs	-3510.00	kJ/mol	NIST Webbook
gf	-233.22	kJ/mol	Joback Method
hf	-327.88	kJ/mol	Joback Method
hfs	-592.00	kJ/mol	NIST Webbook
hfs	-458.30 ± 1.60	kJ/mol	NIST Webbook
hfus	22.32	kJ/mol	Enthalpies of combustion and formation of benzenesulfonamide and some of its derivatives
hvap	71.81	kJ/mol	Joback Method
log10ws	-1.39		Aqueous Solubility Prediction Method

log10ws	-1.34		Estimated Solubility Method
logp	-0.084		Crippen Method
mcvol	119.690	ml/mol	McGowan Method
pc	6841.44	kPa	Joback Method
tb	561.18	K	Joback Method
tc	794.22	K	Joback Method
tf	438.65 ± 0.60	K	NIST Webbook
tf	438.65	K	Aqueous Solubility Prediction Method
tt	437.78	K	Solubility and Thermodynamic Modeling of Sulfanilamide in 12 Mono Solvents and 4 Binary Solvent Mixtures from 278.15 to 318.15 K
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.97	J/mol×K	755.38	Joback Method
cpg	269.49	J/mol×K	561.18	Joback Method
cpg	280.30	J/mol×K	600.02	Joback Method
cpg	290.34	J/mol×K	638.86	Joback Method
cpg	299.63	J/mol×K	677.70	Joback Method
cpg	308.17	J/mol×K	716.54	Joback Method
cpg	323.03	J/mol×K	794.22	Joback Method
cps	220.90	J/mol×K	323.00	NIST Webbook
hfust	23.30	kJ/mol	435.40	NIST Webbook

Sources

Volumetric Properties of Glycine in Aqueous Solutions of Some Sulfa Drugs at (288.15, 298.15, and 308.15) K:	https://www.doi.org/10.1021/je300455e
Interactions between Sulpha Drugs and Magnesium Chloride in Aqueous Solutions at T = (288.15 to 318.15) K: Volumetric and Viscometric Approach:	https://www.doi.org/10.1021/je4002448
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63741&Units=SI
Solubility of p-Aminobenzenesulfonamide in Different Solvents from (283.15 to 325.15) K:	https://www.doi.org/10.1021/je900038m
Solubility of p-Aminobenzenesulfonamide in Supercritical Carbon Dioxide with Acetone Cosolvent:	https://www.doi.org/10.1021/je800700r
Solubility and Thermodynamic Properties of Some Sulpha Drugs in Aqueous Solutions of Sodium Chloride at T = (288.15 to 318.15) K:	https://www.doi.org/10.1021/je900798p
Solubility and Thermodynamic Modeling of Sulfanilamide in 12 Mono Solvents and 4 Binary Solvent Mixtures from 278.15 to 318.15 K:	https://www.doi.org/10.1021/acs.jced.9b00411

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Enthalpies of combustion and formation of benzenesulfonamide and some of its derivatives:	https://www.doi.org/10.1016/j.jct.2011.11.026
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Volumetric approach to the interaction of diglycine in aqueous solutions of sulpha drugs at T = 288.15 to 308.15 K:	https://www.doi.org/10.1016/j.fluid.2012.08.001

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume