Sulfaguanidine

Other names:

((4-Aminophenyl)sulfonyl)guanidine
((p-Aminophenyl)sulfonyl)guanidine
1-((p-Aminophenyl)sulfonyl)guanidine
1-Sulfanilylguanidine
4-Amino-N-(aminoiminomethyl)benzenesulfonamide
4-Amino-N-(diaminomethylene)benzenesulfonamide
4-Aminobenzenesulfonylguanidine
A-307
Abiguanil
Aterian
Benzenesulfonamide, 4-amino-N-(aminoiminomethyl)-
Benzenesulfonamide, 4-amino-N-(diaminomethylene)-
Diacta
Emerin (pharmaceutical)
Ganidan
Guamide
Guanicil
Guanidan
Guanidine, sulfanilyl-
N-1-Amidinosulfanilamide
N-Guanylsulfanilamide
N-p-Aminobenzenesulphonylguanidine monohydrate
N1-Guanidylsulfanilamide
N1-Guanylsulfanilamide
Orgaguanidon
RP 2275
Resulfon
Ruocid
S-Guanidine
Shigatox
Suganyl
Sulfaguamidine
Sulfaguanidin
Sulfaguanil
Sulfaguine
Sulfanilamide, N(sup1)-amidino-
Sulfanilamide, N1-(diaminomethylene)-
Sulfanilamide, N1-amidino-
Sulfanilguanidine
Sulfanilylguanidine

	Sulfentidine
	Sulfoguanidine
	Sulfoguanil
	Sulfoguanyl
	Sulfoguenil
	Sulfoquanidine
	Sulgin
	Sulphaguanidine
	p-Aminobenzenesulfoguanidide
	p-Aminobenzenesulfonylguanidine
Inchi:	InChI=1S/C7H10N4O2S/c8-5-1-3-6(4-2-5)14(12,13)11-7(9)10/h1-4H,8H2,(H4,9,10,11)
InchiKey:	BRBKOPJOKNSWSG-UHFFFAOYSA-N
Formula:	C7H10N4O2S
SMILES:	N=C(N)NS(=O)(=O)c1ccc(N)cc1
Mol. weight [g/mol]:	214.25
CAS:	57-67-0

Physical Properties

Property code	Value	Unit	Source
gf	68.19	kJ/mol	Joback Method
hf	-96.72	kJ/mol	Joback Method
hvap	92.55	kJ/mol	Joback Method
log10ws	-1.98		Aqueous Solubility Prediction Method
log10ws	-1.99		Estimated Solubility Method
logp	-0.559		Crippen Method
mcvol	149.440	ml/mol	McGowan Method
tb	718.57	K	Joback Method
tf	464.65	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.35	J/mol×K	718.57	Joback Method
cpg	82.75	J/mol×K	100.12	Joback Method
cpg	82.75	J/mol×K	100.12	Joback Method

cpg	82.75	J/mol×K	100.12	Joback Method
cpg	82.75	J/mol×K	100.12	Joback Method
cpg	82.75	J/mol×K	100.12	Joback Method
cpg	82.75	J/mol×K	100.12	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57670&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point