Benzenesulfonic acid, 4-amino-

Other names:	4-Amino benzenesulphonic acid
	4-Aminobenzenesulfonic acid
	ANILINE-P-SULFONIC ACID
	Aniline-4-sulfonic acid
	Aniline-p-sulphonic acid
	Kyselina sulfanilova
	NSC 7170
	P-AMINOBENZENESULFONIC ACID
	SULPHANILIC ACID
	Sulfanilic acid
	Sulfanilsaeure
	p-Aminophenylsulfonic acid
	p-Anilinesulfonic acid
Inchi:	InChI=1S/C6H7NO3S/c7-5-1-3-6(4-2-5)11(8,9)10/h1-4H,7H2,(H,8,9,10)
InchiKey:	HVBSAKJJOYLTQU-UHFFFAOYSA-N
Formula:	C6H7NO3S
SMILES:	Nc1ccc(S(=O)(=O)O)cc1
Mol. weight [g/mol]:	173.19
CAS:	121-57-3

Physical Properties

Property code	Value	Unit	Source
chs	-3351.20 ± 0.50	kJ/mol	NIST Webbook
gf	-436.49	kJ/mol	Joback Method
hf	-513.90	kJ/mol	Joback Method
hfs	-612.30 ± 1.00	kJ/mol	NIST Webbook
hfus	25.61	kJ/mol	Joback Method
hvap	77.84	kJ/mol	Joback Method
log10ws	-0.69		Crippen Method
logp	0.516		Crippen Method
mcvol	115.580	ml/mol	McGowan Method
pc	7255.44	kPa	Joback Method
tb	580.83	K	Joback Method
tc	787.92	K	Joback Method

tf	561.10	K	Thermodynamic Models for Determination of the Solubility of Sulfanilic Acid in Different Solvents at Temperatures from (278.15 to 328.15) K
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.80	J/mol×K	580.83	Joback Method
cpg	270.63	J/mol×K	615.34	Joback Method
cpg	278.88	J/mol×K	649.86	Joback Method
cpg	286.56	J/mol×K	684.37	Joback Method
cpg	293.68	J/mol×K	718.89	Joback Method
cpg	300.24	J/mol×K	753.40	Joback Method
cpg	306.24	J/mol×K	787.92	Joback Method

Sources

Thermodynamic Models for Determination of the Solubility of Sulfanilic Acid in Different Solvents at Temperatures from (278.15 to 328.15) K:	https://www.doi.org/10.1021/je500867u
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1881.mol
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Interactions between Sulpha Drugs and Magnesium Chloride in Aqueous Solutions at T = (288.15 to 318.15) K:	https://www.doi.org/10.1021/je4002448
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121573&Units=SI
Volumetric and Viscometric Approach:	https://www.doi.org/10.1021/je900798p
Volumetric and Viscometric Properties of Some Sulpha Drugs in Aqueous Solutions of Sodium Chloride at T = (288.15 to 318.15) K:	

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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
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
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/26-157-9/Benzenesulfonic-acid-4-amino.pdf
Generated by Cheméo on 2024-04-18 13:36:31.849123694 +0000 UTC m=+15736640.769701016.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.