Aminosalicylic Acid

Other names:

2-Hydroxy-4-aminobenzoic acid
3-Hydroxy-4-carboxyaniline
4-ASA
4-Amino-2-hydroxybenzoic acid
4-Aminosalicylic acid
A 1909
Amino-pas
Aminopar
Aminox
Apacil
Apas
Benzoic acid, 4-amino-2-hydroxy-
Deapasil
Entepas
Ferrosan
Gabbropas
Hellipidyl
Kyselina p-aminosalicylova
NIH 2939
NSC 2083
Osacyl
PAS
PAS (acid)
PAS-C
PASK
Pamacyl
Pamisyl
Paramycin
Parasal
Parasalicil
Parasalindon
Pasa
Pasalon
Pasara
Pascorbic
Pasdium
Pasem
Paser
Pasmed
Pasnodia

	Pasolac
	Propasa
	Rezipas
	Salicylic acid, 4-amino-
	Sanipirol-4
	Sanipriol-4
	p-Aminosalicylic acid
	para-Amino salicylic acid
	para-Pas
Inchi:	InChI=1S/C7H7NO3/c8-4-1-2-5(7(10)11)6(9)3-4/h1-3,9H,8H2,(H,10,11)
InchiKey:	WUBBRNOQWQTFEX-UHFFFAOYSA-N
Formula:	C7H7NO3
SMILES:	Nc1ccc(C(=O)O)c(O)c1
Mol. weight [g/mol]:	153.14
CAS:	65-49-6

Physical Properties

Property code	Value	Unit	Source
gf	-243.07	kJ/mol	Joback Method
hf	-371.08	kJ/mol	Joback Method
hfus	24.21	kJ/mol	Joback Method
hvap	81.19	kJ/mol	Joback Method
log10ws	-2.01		Aqueous Solubility Prediction Method
logp	0.673		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	6796.39	kPa	Joback Method
tb	690.42	K	Joback Method
tc	918.13	K	Joback Method
tf	423.65	K	Aqueous Solubility Prediction Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.00	J/mol×K	690.42	Joback Method

cpg	283.98	J/mol×K	728.37	Joback Method
cpg	290.51	J/mol×K	766.32	Joback Method
cpg	296.65	J/mol×K	804.27	Joback Method
cpg	302.48	J/mol×K	842.23	Joback Method
cpg	308.08	J/mol×K	880.18	Joback Method
cpg	313.51	J/mol×K	918.13	Joback Method
hfust	47.90	kJ/mol	406.20	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65496&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of 4-Aminosalicylic Acid in Supercritical Carbon Dioxide and Subcritical 1,1,1,2-Tetrafluoroethane:	https://www.doi.org/10.1021/je5002736
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
vc:	Critical Volume