4-aminobenzoic acid

Other names: benzoic acid, 4-amino-
p-Aminobenzoic acid
Inchi: InChI=1S/C7H7NO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,8H2,(H,9,10)
InchiKey: ALYNCZNDIQEVRV-UHFFFAOYSA-N
Formula: C7H7NO2
SMILES: Nc1ccc(C(=O)O)cc1
Mol. weight [g/mol]: 137.14
CAS: 150-13-0

Physical Properties

Property code	Value	Unit	Source
affp	864.70	kJ/mol	NIST Webbook
basg	832.30	kJ/mol	NIST Webbook
chs	-3342.00 ± 0.40	kJ/mol	NIST Webbook
chs	-3345.00 ± 1.50	kJ/mol	NIST Webbook
chs	-3427.00	kJ/mol	NIST Webbook
gf	-88.45	kJ/mol	Joback Method
hf	-293.90 ± 4.10	kJ/mol	NIST Webbook
hfs	-328.30	kJ/mol	NIST Webbook
hfs	-413.00 ± 0.40	kJ/mol	NIST Webbook
hfs	-410.00 ± 1.70	kJ/mol	NIST Webbook
hfus	25.00	kJ/mol	Solution thermodynamics of pyrazinamide, isoniazid, and p-aminobenzoic acid in buffers and octanol
hsub	116.10 ± 3.70	kJ/mol	NIST Webbook
hsub	116.00 ± 3.70	kJ/mol	NIST Webbook
hsub	116.10 ± 3.70	kJ/mol	NIST Webbook
hvap	68.18	kJ/mol	Joback Method
ie	8.40	eV	NIST Webbook
ie	8.40 ± 0.20	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
log10ws	-0.63		Aqueous Solubility Prediction Method
log10ws	-1.37		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.967		Crippen Method

mcvol	103.150	ml/mol	McGowan Method
pc	5390.71	kPa	Joback Method
rinpol	1547.00		NIST Webbook
tb	609.80	K	Joback Method
tc	828.81	K	Joback Method
tf	461.40 ± 0.60	K	NIST Webbook
tf	461.68	K	Aqueous Solubility Prediction Method
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.91	J/mol×K	792.31	Joback Method
cpg	240.14	J/mol×K	609.80	Joback Method
cpg	248.38	J/mol×K	646.30	Joback Method
cpg	256.05	J/mol×K	682.80	Joback Method
cpg	263.18	J/mol×K	719.31	Joback Method
cpg	269.79	J/mol×K	755.81	Joback Method
cpg	281.56	J/mol×K	828.81	Joback Method
cps	177.80	J/mol×K	298.00	NIST Webbook
cps	187.40	J/mol×K	323.00	NIST Webbook
hfust	20.92	kJ/mol	461.40	NIST Webbook
hfust	22.62	kJ/mol	458.70	NIST Webbook
hfust	24.50	kJ/mol	459.20	NIST Webbook
hfust	20.92	kJ/mol	461.40	NIST Webbook
hfust	20.92	kJ/mol	461.40	NIST Webbook
hsubt	114.00 ± 3.50	kJ/mol	378.00	NIST Webbook
hsubt	112.00 ± 1.00	kJ/mol	373.00	NIST Webbook
sfust	45.30	J/mol×K	461.40	NIST Webbook

Sources

Solution thermodynamics of pyrazinamide, isoniazid, and p-aminobenzoic acid in buffers and octanol:	https://www.doi.org/10.1016/j.jct.2015.08.022
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Mixed Solubilities of 5-Sulfosalicylic Acid and p-Aminobenzoic Acid in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je700159k
Solubility of mixed solids in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.fluid.2006.11.002
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C150130&Units=SI

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume