Benzoic acid, 3-amino-

Other names:	3-aminobenzoic acid
	3-carboxyaniline
	Aniline-3-carboxylic acid
	Maba
	benzoic acid, m-amino-
	m-Carboxyaniline
	m-aminobenzoic acid
Inchi:	InChI=1S/C7H7NO2/c8-6-3-1-2-5(4-6)7(9)10/h1-4H,8H2,(H,9,10)
InchiKey:	XFDUHJPVQKIXHO-UHFFFAOYSA-N
Formula:	C7H7NO2
SMILES:	Nc1cccc(C(=O)O)c1
Mol. weight [g/mol]:	137.14
CAS:	99-05-8

Physical Properties

Property code	Value	Unit	Source
affp	864.70	kJ/mol	NIST Webbook
basg	832.30	kJ/mol	NIST Webbook
chs	-3344.00 ± 0.40	kJ/mol	NIST Webbook
chs	-3337.60 ± 1.30	kJ/mol	NIST Webbook
gf	-88.45	kJ/mol	Joback Method
hf	-289.30 ± 3.60	kJ/mol	NIST Webbook
hfs	-417.30 ± 1.60	kJ/mol	NIST Webbook
hfs	-411.00 ± 0.40	kJ/mol	NIST Webbook
hfus	18.42	kJ/mol	Joback Method
hsub	128.00 ± 3.20	kJ/mol	NIST Webbook
hsub	128.00 ± 3.20	kJ/mol	NIST Webbook
hvap	68.18	kJ/mol	Joback Method
ie	8.30	eV	NIST Webbook
ie	8.40 ± 0.20	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
log10ws	-1.17		Crippen Method
logp	0.967		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	5390.71	kPa	Joback Method
tb	609.80	K	Joback Method
tc	828.81	K	Joback Method

tf	452.90 ± 0.60	K	NIST Webbook
tf	447.20	K	Solubility of 3-Aminobenzoic Acid in Supercritical Carbon Dioxide Modified by Ethanol
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	162.80	J/mol×K	298.00	NIST Webbook
cps	179.90	J/mol×K	323.00	NIST Webbook
hfust	21.84	kJ/mol	452.90	NIST Webbook
hfust	33.70	kJ/mol	445.70	NIST Webbook
hfust	21.84	kJ/mol	452.90	NIST Webbook
hfust	21.84	kJ/mol	452.90	NIST Webbook
hsubt	122.00 ± 3.00	kJ/mol	378.00	NIST Webbook
hsubt	122.00 ± 1.00	kJ/mol	374.80	NIST Webbook
sfust	48.20	J/mol×K	452.90	NIST Webbook

Sources

Binary and ternary solubility of amino- and nitro-benzoic acids in supercritical carbon dioxide: https://www.doi.org/10.1016/j.fluid.2013.01.021

Solubility of 3-Aminobenzoic Acid in Supercritical Carbon Dioxide Modified by Ethanol: https://www.doi.org/10.1021/je4000845

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C99058&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume