Acetophenone, 4'-amino-

Other names:	1-(4-Aminophenyl)ethanone
	1-Acetyl-4-aminobenzene
	4'-Aminoacetophenone
	4-Acetylaniline
	4-Aminoacetophenone
	4-acetylphenylamine
	Acetophenone, p-amino-
	Ethanone, 1-(4-aminophenyl)-
	NSC 3242
	USAF EK-631
	aniline, 4-acetyl-
	p-Acetylaniline
	p-Aminoacetofenonu
	p-Aminoacetophenone
	p-Aminoacetylbenzene
Inchi:	InChI=1S/C8H9NO/c1-6(10)7-2-4-8(9)5-3-7/h2-5H,9H2,1H3
InchiKey:	GPRYKVSEZCQIHD-UHFFFAOYSA-N
Formula:	C8H9NO
SMILES:	CC(=O)c1ccc(N)cc1
Mol. weight [g/mol]:	135.16
CAS:	99-92-3

Physical Properties

Property code	Value	Unit	Source
affp	908.80	kJ/mol	NIST Webbook
basg	877.00	kJ/mol	NIST Webbook
chs	-4726.70 ± 0.80	kJ/mol	NIST Webbook
chs	-4729.64 ± 0.84	kJ/mol	NIST Webbook
chs	-4252.20 ± 0.40	kJ/mol	NIST Webbook
gf	56.79	kJ/mol	Joback Method
hf	-62.18	kJ/mol	Joback Method
hfs	-182.00 ± 0.40	kJ/mol	NIST Webbook
hfus	19.56	kJ/mol	Solid liquid equilibria for binary mixtures of N-phenylacetamide with 4-aminoacetophenone, 3-hydroxyacetophenone and 4-hydroxyacetophenone

hvap	53.73	kJ/mol	Joback Method
ie	8.27	eV	NIST Webbook
ie	8.17 ± 0.02	eV	NIST Webbook
ie	8.30 ± 0.10	eV	NIST Webbook
ie	7.80 ± 0.10	eV	NIST Webbook
log10ws	-1.61		Aqueous Solubility Prediction Method
logp	1.471		Crippen Method
mcvol	111.370	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
rinpol	1440.00		NIST Webbook
rinpol	1440.00		NIST Webbook
ripol	2181.00		NIST Webbook
ripol	2181.00		NIST Webbook
tb	567.00 ± 1.00	K	NIST Webbook
tb	567.20	K	NIST Webbook
tc	774.37	K	Joback Method
tf	379.15 ± 1.00	K	NIST Webbook
tf	379.00	K	NIST Webbook
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.00	J/mol×K	618.46	Joback Method
cpg	274.92	J/mol×K	657.43	Joback Method
cpg	284.13	J/mol×K	696.41	Joback Method
cpg	292.68	J/mol×K	735.39	Joback Method
cpg	242.96	J/mol×K	540.50	Joback Method
cpg	254.36	J/mol×K	579.48	Joback Method
cpg	300.60	J/mol×K	774.37	Joback Method
hfust	19.60	kJ/mol	378.20	NIST Webbook
hfust	38.00	kJ/mol	379.20	NIST Webbook
hfust	38.00	kJ/mol	379.20	NIST Webbook
hsubt	92.70	kJ/mol	326.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99923&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solid liquid equilibria for binary mixtures of N-phenylacetamide with 4-aminoacetophenone, 3-hydroxyacetophenone and 4-hydroxyacetophenone:	https://www.doi.org/10.1016/j.fluid.2005.03.023

Legend

affp:	Proton affinity
basg:	Gas basicity
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
hfust:	Enthalpy of fusion at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume