3-Aminoacetophenone

Other names:	1-(3-Aminophenyl)ethanone
	3'-Aminoacetophenone
	3-Acetylaniline
	3-Acetylphenylamine
	3-Aminoacetofenon
	Acetophenone, 3'-amino-
	Acetophenone, m-amino-
	Ethanone, 1-(3-aminophenyl)-
	NSC 7637
	m-Acetylaniline
	m-Aminoacetophenone
	m-Aminoacetylbenzene
	«beta»-Aminoacetophenone
	Â«betaÂ»-Aminoacetophenone
Inchi:	InChI=1S/C8H9NO/c1-6(10)7-3-2-4-8(9)5-7/h2-5H,9H2,1H3
InchiKey:	CKQHAYFOPRIUOM-UHFFFAOYSA-N
Formula:	C8H9NO
SMILES:	CC(=O)c1cccc(N)c1
Mol. weight [g/mol]:	135.16
CAS:	99-03-6

Physical Properties

Property code	Value	Unit	Source
chs	-4261.00 ± 0.40	kJ/mol	NIST Webbook
gf	56.79	kJ/mol	Joback Method
hf	-62.18	kJ/mol	Joback Method
hfs	-173.00 ± 0.40	kJ/mol	NIST Webbook
hfus	16.92	kJ/mol	Joback Method
hvap	53.73	kJ/mol	Joback Method
ie	8.60 ± 0.20	eV	NIST Webbook
ie	8.09 ± 0.05	eV	NIST Webbook
log10ws	-1.28		Aqueous Solubility Prediction Method
logp	1.471		Crippen Method
mcvol	111.370	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
rinpol	1409.00		NIST Webbook

ripol	2518.00		NIST Webbook
ripol	2518.00		NIST Webbook
ripol	2518.00		NIST Webbook
tb	562.70	K	NIST Webbook
tc	774.37	K	Joback Method
tf	370.32	K	Aqueous Solubility Prediction Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.96	J/mol×K	540.50	Joback Method
cpg	254.36	J/mol×K	579.48	Joback Method
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	300.60	J/mol×K	774.37	Joback Method
hfust	29.00	kJ/mol	371.20	NIST Webbook
hfust	29.00	kJ/mol	371.20	NIST Webbook

Sources

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=C99036&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
hfust:	Enthalpy of fusion 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