Ethanone, 1-(2-aminophenyl)-

Other names:	Acetophenone, 2'-amino-
	o-Aminoacetophenone
	o-Aminoacetylbenzene
	2-Acetylaniline
	2'-Aminoacetophenone
	2-Aminoacetophenone
	o-Aminophenyl methyl ketone
	1-Acetyl-2-aminobenzene
	ortho-Aminoacetophenone
	2-Acetylphenylamine
	NSC 8820
	o-Acetylaniline
	1-(2-aminophenyl)ethanone
	ortho-aminoacetophenone (2'-aminoacetophenone)
Inchi:	InChI=1S/C8H9NO/c1-6(10)7-4-2-3-5-8(7)9/h2-5H,9H2,1H3
InchiKey:	GTDQGKWDWVUKTI-UHFFFAOYSA-N
Formula:	C8H9NO
SMILES:	CC(=O)c1ccccc1N
Mol. weight [g/mol]:	135.16
CAS:	551-93-9

Physical Properties

Property code	Value	Unit	Source
gf	56.79	kJ/mol	Joback Method
hf	-62.18	kJ/mol	Joback Method
hfus	16.92	kJ/mol	Joback Method
hvap	53.73	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.471		Crippen Method
mcvol	111.370	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
rinpol	1315.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1285.00		NIST Webbook

rinpol	1262.00	NIST Webbook
rinpol	1262.00	NIST Webbook
rinpol	1262.00	NIST Webbook
rinpol	1300.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1292.00	NIST Webbook
rinpol	1260.00	NIST Webbook
rinpol	1325.00	NIST Webbook
rinpol	1299.00	NIST Webbook
rinpol	1302.00	NIST Webbook
rinpol	1300.00	NIST Webbook
rinpol	1306.00	NIST Webbook
rinpol	1306.00	NIST Webbook
rinpol	1292.00	NIST Webbook
rinpol	1316.00	NIST Webbook
rinpol	1310.00	NIST Webbook
rinpol	1308.00	NIST Webbook
rinpol	1308.00	NIST Webbook
rinpol	1308.00	NIST Webbook
rinpol	1306.00	NIST Webbook
rinpol	1307.00	NIST Webbook
rinpol	1322.00	NIST Webbook
rinpol	1320.00	NIST Webbook
rinpol	1299.00	NIST Webbook
rinpol	1296.00	NIST Webbook
rinpol	1318.00	NIST Webbook
rinpol	1315.00	NIST Webbook
rinpol	1308.00	NIST Webbook
rinpol	1300.00	NIST Webbook
rinpol	1285.00	NIST Webbook
rinpol	1315.00	NIST Webbook
rinpol	1265.00	NIST Webbook
rinpol	1288.00	NIST Webbook
rinpol	1288.00	NIST Webbook
ripol	2228.00	NIST Webbook
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ripol	2200.00	NIST Webbook
ripol	2210.00	NIST Webbook
ripol	2181.00	NIST Webbook
ripol	2200.00	NIST Webbook

ripol	2242.00		NIST Webbook
ripol	2223.00		NIST Webbook
ripol	2227.00		NIST Webbook
ripol	2234.00		NIST Webbook
ripol	2238.00		NIST Webbook
ripol	2228.00		NIST Webbook
ripol	2227.00		NIST Webbook
ripol	2252.00		NIST Webbook
ripol	2187.00		NIST Webbook
ripol	2213.00		NIST Webbook
ripol	2225.00		NIST Webbook
ripol	2184.00		NIST Webbook
ripol	2222.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2237.00		NIST Webbook
ripol	2270.00		NIST Webbook
ripol	2218.00		NIST Webbook
ripol	2222.00		NIST Webbook
ripol	2229.00		NIST Webbook
ripol	2204.00		NIST Webbook
ripol	2222.00		NIST Webbook
ripol	2202.00		NIST Webbook
ripol	2223.00		NIST Webbook
ripol	2225.00		NIST Webbook
ripol	2182.00		NIST Webbook
ripol	2240.00		NIST Webbook
ripol	2202.00		NIST Webbook
tb	540.50	K	Joback Method
tc	774.37	K	Joback Method
tf	352.05	K	Joback 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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	343.70	K	0.40	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C551939&Units=SI

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
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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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