1-Butanone, 1-(4-aminophenyl)-

Other names:	Butyrophenone, 4'-amino- p-Aminobutyrophenone 4'-Aminobutyrophenone 1-(4-Aminophenyl)-1-butanone
Inchi:	InChI=1S/C10H13NO/c1-2-3-10(12)8-4-6-9(11)7-5-8/h4-7H,2-3,11H2,1H3
InchiKey:	CYCSOZSEBPZGPC-UHFFFAOYSA-N
Formula:	C10H13NO
SMILES:	CCCC(=O)c1ccc(N)cc1
Mol. weight [g/mol]:	163.22
CAS:	1688-71-7

Physical Properties

Property code	Value	Unit	Source
gf	73.63	kJ/mol	Joback Method
hf	-103.46	kJ/mol	Joback Method
hfus	22.10	kJ/mol	Joback Method
hvap	58.18	kJ/mol	Joback Method
ie	8.00 ± 0.20	eV	NIST Webbook
log10ws	-2.60		Crippen Method
logp	2.252		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
tb	586.26	K	Joback Method
tc	811.30	K	Joback Method
tf	374.59	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.24	J/mol×K	586.26	Joback Method
cpg	346.54	J/mol×K	623.77	Joback Method
cpg	358.98	J/mol×K	661.27	Joback Method
cpg	370.61	J/mol×K	698.78	Joback Method

cpg	381.46	J/mol×K	736.29	Joback Method
cpg	391.57	J/mol×K	773.79	Joback Method
cpg	400.96	J/mol×K	811.30	Joback Method

Sources

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=C1688717&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume