1-(3-Aminophenyl)-1-butanone

Inchi: InChI=1S/C10H13NO/c1-2-4-10(12)8-5-3-6-9(11)7-8/h3,5-7H,2,4,11H2,1H3
InchiKey: JQHVNKSERJZHCO-UHFFFAOYSA-N
Formula: C10H13NO
SMILES: CCCC(=O)c1cccc(N)c1
Mol. weight [g/mol]: 163.22
CAS: 2034-41-5

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	8.10 ± 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:	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=C2034415&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
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