1-Propanone, 1-(4-aminophenyl)-

Other names:	1-(4-Aminophenyl)-1-propanone
	4'-Aminopropiophenone
	4-Aminopropiophenone
	4-Propionylaniline
	Ethyl p-aminophenyl ketone
	NSC 3187
	PAPP
	Para-aminopropiophenone
	Propiophenone, 4'-amino-
	USAF uctl-1856
	p-Aminopropiophenone
Inchi:	InChI=1S/C9H11NO/c1-2-9(11)7-3-5-8(10)6-4-7/h3-6H,2,10H2,1H3
InchiKey:	FSWXOANXOQPCFF-UHFFFAOYSA-N
Formula:	C9H11NO
SMILES:	CCC(=O)c1ccc(N)cc1
Mol. weight [g/mol]:	149.19
CAS:	70-69-9

Physical Properties

Property code	Value	Unit	Source
gf	65.21	kJ/mol	Joback Method
hf	-82.82	kJ/mol	Joback Method
hfus	19.51	kJ/mol	Joback Method
hvap	55.95	kJ/mol	Joback Method
log10ws	-2.63		Aqueous Solubility Prediction Method
logp	1.861		Crippen Method
mcvol	125.460	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
tb	563.38	K	Joback Method
tc	792.76	K	Joback Method
tf	363.32	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.22	J/mol×K	563.38	Joback Method
cpg	299.64	J/mol×K	601.61	Joback Method
cpg	311.25	J/mol×K	639.84	Joback Method
cpg	322.09	J/mol×K	678.07	Joback Method
cpg	332.18	J/mol×K	716.30	Joback Method
cpg	341.56	J/mol×K	754.53	Joback Method
cpg	350.26	J/mol×K	792.76	Joback Method

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=C70699&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume