«beta»-(4-Aminophenyl)propionic acid

Other names:	«beta»-(p-Aminophenyl)propionic acid
	p-Aminohydrocinnamic acid
	Benzenepropanoic acid, 4-amino-
	3-(p-aminophenyl)propionic acid
Inchi:	InChI=1S/C9H11NO2/c10-8-4-1-7(2-5-8)3-6-9(11)12/h1-2,4-5H,3,6,10H2,(H,11,12)
InchiKey:	WXOHKMNWMKZMND-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	Nc1ccc(CCC(=O)O)cc1
Mol. weight [g/mol]:	165.19
CAS:	2393-17-1

Physical Properties

Property code	Value	Unit	Source
gf	-71.61	kJ/mol	Joback Method
hf	-235.05	kJ/mol	Joback Method
hfus	23.60	kJ/mol	Joback Method
hvap	72.63	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.286		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	4140.93	kPa	Joback Method
tb	655.56	K	Joback Method
tc	867.32	K	Joback Method
tf	424.14	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.06	J/mol×K	655.56	Joback Method
cpg	343.03	J/mol×K	690.85	Joback Method
cpg	352.35	J/mol×K	726.15	Joback Method
cpg	361.05	J/mol×K	761.44	Joback Method
cpg	369.15	J/mol×K	796.73	Joback Method

cpg	376.69	J/mol×K	832.03	Joback Method
cpg	383.70	J/mol×K	867.32	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=C2393171&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume