

Benzeneacetic acid, 4-amino-

Other names:	Acetic acid, (p-aminophenyl)- p-Aminophenylacetic acid 4-Aminobenzeneacetic acid 4-Aminophenylacetic acid (para-Aminophenyl)acetic acid p-Amino-«alpha»-toluic acid 4-Carboxymethylaniline NSC 7929
Inchi:	InChI=1S/C8H9NO2/c9-7-3-1-6(2-4-7)5-8(10)11/h1-4H,5,9H2,(H,10,11)
InchiKey:	CSEWAUGPAQPMDC-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	<chem>Nc1ccc(CC(=O)O)cc1</chem>
Mol. weight [g/mol]:	151.16
CAS:	1197-55-3

Physical Properties

Property code	Value	Unit	Source
gf	-80.03	kJ/mol	Joback Method
hf	-214.41	kJ/mol	Joback Method
hfus	21.01	kJ/mol	Joback Method
hvap	70.41	kJ/mol	Joback Method
log10ws	-1.01		Crippen Method
logp	0.896		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4704.19	kPa	Joback Method
tb	632.68	K	Joback Method
tc	847.92	K	Joback Method
tf	412.87	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.76	J/molxK	812.05	Joback Method

cpg	285.81	J/mol×K	632.68	Joback Method
cpg	294.96	J/mol×K	668.55	Joback Method
cpg	303.51	J/mol×K	704.43	Joback Method
cpg	311.48	J/mol×K	740.30	Joback Method
cpg	318.88	J/mol×K	776.17	Joback Method
cpg	332.13	J/mol×K	847.92	Joback Method
hfust	42.70	kJ/mol	468.20	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=C1197553&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
hfust:	Enthalpy of fusion at a given temperature
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

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