Hippuric acid

Other names:	2-(benzoylamino)acetic acid
	2-Benzamidoacetic acid
	Acetic acid, (benzoylamino)-
	Acido ippurico
	Benzamidoacetic acid
	Benzenecarboxamide, N-carboxymethyl-
	Benzoylaminoacetic acid
	Benzoylglycin
	Benzoylglycine
	Benzoylglycocoll
	Glycine, N-benzoyl-
	N-Benzoylglycine
	NSC 9982
	Phenylcarbonylaminoacetic acid
Inchi:	InChI=1S/C9H9NO3/c11-8(12)6-10-9(13)7-4-2-1-3-5-7/h1-5H,6H2,(H,10,13)(H,11,12)
InchiKey:	QIAFMBKCNZACKA-UHFFFAOYSA-N
Formula:	C9H9NO3
SMILES:	O=C(O)CNC(=O)c1ccccc1
Mol. weight [g/mol]:	179.17
CAS:	495-69-2

Physical Properties

Property code	Value	Unit	Source
chl	-4217.80 ± 1.60	kJ/mol	NIST Webbook
gf	-167.96	kJ/mol	Joback Method
hf	-316.48	kJ/mol	Joback Method
hfs	-608.90 ± 1.70	kJ/mol	NIST Webbook
hfs	-611.10 ± 1.30	kJ/mol	NIST Webbook
hfs	-607.50 ± 1.90	kJ/mol	NIST Webbook
hfs	-609.53	kJ/mol	NIST Webbook
hfus	25.49	kJ/mol	Joback Method
hvap	74.51	kJ/mol	Joback Method
log10ws	-1.71		Aqueous Solubility Prediction Method
logp	0.501		Crippen Method
mcvol	132.900	ml/mol	McGowan Method
pc	4328.25	kPa	Joback Method

ss	239.30	J/mol×K	NIST Webbook
tb	682.09	K	Joback Method
tc	892.20	K	Joback Method
tf	474.32	K	Aqueous Solubility Prediction Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.18	J/mol×K	682.09	Joback Method
cpg	346.36	J/mol×K	717.11	Joback Method
cpg	354.86	J/mol×K	752.13	Joback Method
cpg	362.73	J/mol×K	787.15	Joback Method
cpg	370.00	J/mol×K	822.16	Joback Method
cpg	376.69	J/mol×K	857.18	Joback Method
cpg	382.84	J/mol×K	892.20	Joback Method
cps	217.00	J/mol×K	298.15	NIST Webbook
cps	214.35	J/mol×K	298.40	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Measurement and Correlation of the Solubility of Pyrimethanil in Seven Monosolvents and Two Different Binary Mixed Solvents: https://www.doi.org/10.1021/acs.jced.8b00124

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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=C495692&Units=SI

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

cps: Solid phase heat capacity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfs:	Solid phase 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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume