

2-Phenylglycine

Other names:	Benzeneacetic acid, «alpha»-amino-, (.+/-)- (.+/-)-«alpha»-Phenylglycine DL-«alpha»-Aminophenylacetic acid DL-«alpha»-Phenylglycine DL-Phenylglycine DL-2-Phenylglycine Glycine, 2-phenyl-, DL- 2-Amino-2-phenylacetic acid Benzeneacetic acid, alpha-amino- NSC 24619 NSC 32070 «alpha»-Aminobenzeneacetic ac «alpha»-Aminophenylacetic acid «alpha»-Phenylglycine
Inchi:	InChI=1S/C8H9NO2/c9-7(8(10)11)6-4-2-1-3-5-6/h1-5,7H,9H2,(H,10,11)
InchiKey:	ZGUNAGUHMKGQNY-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	NC(C(=O)O)c1ccccc1
Mol. weight [g/mol]:	151.16
CAS:	2835-06-5

Physical Properties

Property code	Value	Unit	Source
chs	-4009.00	kJ/mol	NIST Webbook
gf	-72.84	kJ/mol	Joback Method
hf	-208.22	kJ/mol	Joback Method
hfus	17.88	kJ/mol	Joback Method
hvap	69.36	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	0.771		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4856.20	kPa	Joback Method
tb	627.26	K	Joback Method
tc	845.92	K	Joback Method
tf	385.35	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.79	J/mol×K	627.26	Joback Method
cpg	297.38	J/mol×K	663.70	Joback Method
cpg	306.27	J/mol×K	700.15	Joback Method
cpg	314.51	J/mol×K	736.59	Joback Method
cpg	322.13	J/mol×K	773.03	Joback Method
cpg	329.16	J/mol×K	809.48	Joback Method
cpg	335.63	J/mol×K	845.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2835065&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
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

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