

N-Phenylglycine

Other names:	Anilinoacetic acid Glycine, N-phenyl-
Inchi:	InChI=1S/C8H9NO2/c10-8(11)6-9-7-4-2-1-3-5-7/h1-5,9H,6H2,(H,10,11)
InchiKey:	NPKSPKHJBVJUKB-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	O=C(O)CNc1ccccc1
Mol. weight [g/mol]:	151.16
CAS:	103-01-5

Physical Properties

Property code	Value	Unit	Source
chs	-4053.20	kJ/mol	NIST Webbook
chs	-4051.00	kJ/mol	NIST Webbook
chs	-4037.60 ± 0.22	kJ/mol	NIST Webbook
gf	-47.46	kJ/mol	Joback Method
hf	-268.70 ± 2.10	kJ/mol	NIST Webbook
hfs	-396.71 ± 0.57	kJ/mol	NIST Webbook
hfus	21.30	kJ/mol	Joback Method
hsub	128.00 ± 2.00	kJ/mol	NIST Webbook
hsub	128.00 ± 2.00	kJ/mol	NIST Webbook
hvap	65.54	kJ/mol	Joback Method
log10ws	-1.00		Crippen Method
logp	1.183		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4522.49	kPa	Joback Method
tb	605.34	K	Joback Method
tc	811.80	K	Joback Method
tf	369.75	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.30	J/mol×K	777.39	Joback Method

cpg	280.01	J/mol×K	605.34	Joback Method
cpg	289.70	J/mol×K	639.75	Joback Method
cpg	298.74	J/mol×K	674.16	Joback Method
cpg	307.16	J/mol×K	708.57	Joback Method
cpg	315.01	J/mol×K	742.98	Joback Method
cpg	329.07	J/mol×K	811.80	Joback Method
cps	176.60	J/mol×K	298.15	NIST Webbook
hsubt	0.13	kJ/mol	298.15	NIST Webbook
hsubt	114.10 ± 1.00	kJ/mol	365.40	NIST Webbook
ssubt	0.43	J/mol×K	298.15	NIST Webbook

Sources

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=C103015&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid 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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
ssubt:	Entropy of sublimation at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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