N-Phenyliminodiacetic acid

Other names: Acetic acid,1-phenyliminodi-
Glycine, N-(carboxymethyl)-N-phenyl-
Inchi: InChI=1S/C10H11NO4/c12-9(13)6-11(7-10(14)15)8-4-2-1-3-5-8/h1-5H,6-7H2,(H,12,13)(H
InchiKey: GQBWTAGIANQVGB-UHFFFAOYSA-N
Formula: C10H11NO4
SMILES: O=C(O)CN(CC(=O)O)c1ccccc1
Mol. weight [g/mol]: 209.20
CAS: 1137-73-1

Physical Properties

Property code	Value	Unit	Source
gf	-274.97	kJ/mol	Joback Method
hf	-475.29	kJ/mol	Joback Method
hfus	30.09	kJ/mol	Joback Method
hvap	89.02	kJ/mol	Joback Method
log10ws	-0.41		Crippen Method
logp	0.662		Crippen Method
mcvol	152.860	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
tb	759.42	K	Joback Method
tc	955.47	K	Joback Method
tf	482.85	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.11	J/mol×K	759.42	Joback Method
cpg	429.46	J/mol×K	792.09	Joback Method
cpg	437.20	J/mol×K	824.77	Joback Method
cpg	444.39	J/mol×K	857.44	Joback Method
cpg	451.06	J/mol×K	890.12	Joback Method
cpg	457.24	J/mol×K	922.79	Joback Method
cpg	462.97	J/mol×K	955.47	Joback Method

Sources

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=C1137731&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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