1,2-Ethanediamine, N-phenyl-

Other names:	Ethylenediamine, N-phenyl-
	Benzenamine, N-(2-aminoethyl)-
	N-(2-Aminoethyl)aniline
	N-Phenylethylenediamine
	N-Phenyl-1,2-ethanediamine
Inchi:	InChI=1S/C8H12N2/c9-6-7-10-8-4-2-1-3-5-8/h1-5,10H,6-7,9H2
InchiKey:	OCIDXARMXNJACB-UHFFFAOYSA-N
Formula:	C8H12N2
SMILES:	NCCNc1ccccc1
Mol. weight [g/mol]:	136.19
CAS:	1664-40-0

Physical Properties

Property code	Value	Unit	Source
gf	284.73	kJ/mol	Joback Method
hf	115.34	kJ/mol	Joback Method
hfus	20.81	kJ/mol	Joback Method
hvap	52.75	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.057		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
rinpol	1329.60		NIST Webbook
tb	536.20	K	NIST Webbook
tc	755.23	K	Joback Method
tf	342.26	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.18	J/mol×K	531.82	Joback Method
cpg	286.35	J/mol×K	569.06	Joback Method
cpg	298.65	J/mol×K	606.29	Joback Method

cpg	310.13	J/mol×K	643.53	Joback Method
cpg	320.84	J/mol×K	680.76	Joback Method
cpg	330.80	J/mol×K	718.00	Joback Method
cpg	340.06	J/mol×K	755.23	Joback Method

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=C1664400&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume