1,2-Ethanediamine, N-(phenylmethyl)-

Other names: N-Benzylethylenediamine
Ethylenediamine, N-benzyl-
Inchi: InChI=1S/C9H14N2/c10-6-7-11-8-9-4-2-1-3-5-9/h1-5,11H,6-8,10H2
InchiKey: ACYBVNYNIZTUIL-UHFFFAOYSA-N
Formula: C9H14N2
SMILES: NCCNCc1ccccc1
Mol. weight [g/mol]: 150.22
CAS: 4152-09-4

Physical Properties

Property code	Value	Unit	Source
gf	293.15	kJ/mol	Joback Method
hf	94.70	kJ/mol	Joback Method
hfus	23.40	kJ/mol	Joback Method
hvap	54.98	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	0.735		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
tb	554.70	K	Joback Method
tc	774.17	K	Joback Method
tf	353.53	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.46	J/mol×K	554.70	Joback Method
cpg	332.50	J/mol×K	591.28	Joback Method
cpg	345.64	J/mol×K	627.86	Joback Method
cpg	357.92	J/mol×K	664.44	Joback Method
cpg	369.40	J/mol×K	701.01	Joback Method
cpg	380.10	J/mol×K	737.59	Joback Method
cpg	390.07	J/mol×K	774.17	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=C4152094&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