Benzenepropanamine

Other names:	1-Amino-3-phenylpropane
	3-Phenyl-1-aminopropane
	3-Phenyl-1-propanamine
	3-Phenyl-1-propylamine
	3-Phenyl-n-propylamine
	3-Phenylpropanamine
	3-Phenylpropylamine
	Hydrocinnamylamine
	NSC 87080
	Propylamine, 3-phenyl-
	«gamma»-Phenyl-n-propylamine
	«gamma»-Phenylpropylamine
	Â«gammaÂ»-Phenyl-n-propylamine
	Â«gammaÂ»-Phenylpropylamine
Inchi:	InChI=1S/C9H13N/c10-8-4-7-9-5-2-1-3-6-9/h1-3,5-6H,4,7-8,10H2
InchiKey:	LYUQWQRTDLVQGA-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	NCCCc1ccccc1
Mol. weight [g/mol]:	135.21
CAS:	2038-57-5

Physical Properties

Property code	Value	Unit	Source
basg	920.00 ± 8.00	kJ/mol	NIST Webbook
gf	203.76	kJ/mol	Joback Method
hf	41.23	kJ/mol	Joback Method
hfus	18.30	kJ/mol	Joback Method
hvap	48.55	kJ/mol	Joback Method
ie	8.89 ± 0.12	eV	NIST Webbook
log10ws	-2.13		Crippen Method
logp	1.578		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
rinpol	1205.00		NIST Webbook
rinpol	1205.00		NIST Webbook
tb	494.20	K	NIST Webbook
tc	723.91	K	Joback Method

tf	300.87	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.59	J/mol×K	687.35	Joback Method
cpg	271.45	J/mol×K	504.53	Joback Method
cpg	285.54	J/mol×K	541.09	Joback Method
cpg	298.76	J/mol×K	577.66	Joback Method
cpg	311.15	J/mol×K	614.22	Joback Method
cpg	322.74	J/mol×K	650.78	Joback Method
cpg	343.71	J/mol×K	723.91	Joback Method
cpl	265.59	J/mol×K	298.15	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46446e+01
Coeff. B	-4.16770e+03
Coeff. C	-7.85240e+01
Temperature range (K), min.	368.81
Temperature range (K), max.	525.07

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2038575&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

basg:	Gas basicity
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume