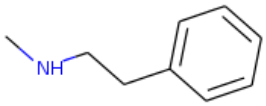
Benzeneethanamine, N-methyl-

Other names: (2-Phenylethyl)methylamine; 1-Phenyl-2-methylamino-aethan; 1-Phenyl-2-methylaminoethane; N-(Phenylethyl)methylamine; N-Methyl-2-phenylethylamine; N-Methyl-N-(2-phenylethyl)amine; N-Methyl-«beta»-phenethylamine; N-Methyl-«beta»-phenylaethylamin; N-Methyl-«beta»-phenylethylamine; N-Methylbenzeneethanamine; N-Methylphenethylamine; N-Methylphenylethylamine; N-Phenethylmethylamine; NSC 113957; Phenethylamine, N-methyl-; WIN 5553; «alpha»-Phenyl-«beta»-methylaminoethane.



InChI: InChI=1S/C9H13N/c1-10-8-7-9-5-3-2-4-6-9/h2-6,10H,7-8H2,1H3

InChI Key: SASNBVQSOZSTPD-UHFFFAOYSA-N

Formula: C9H13N

SMILES: CNCCc1ccccc1

Molecular Weight: 135.21

CAS: 589-08-2

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	226.70	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	60.91	kJ/mol	Joback Method
$\Delta_{fus} H°$	18.21	kJ/mol	Joback Method
$\Delta_{vap} H°$	44.34	kJ/mol	Joback Method
IE	8.40	eV	NIST Webbook
IE	8.66 ± 0.20	eV	NIST Webbook
$logP_{oct/wat}$	1.449		Crippen Method
P_c	3310.55	kPa	Joback Method
T_{boil}	476.20	K	NIST Webbook
T_c	691.55	K	Joback Method
T_{fus}	270.27	K	Joback Method
V_c	0.467	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	260.33	J/mol×K	482.17	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H13N/c1-10-8-7-9-5-3-2-4-6-9/h2-6,10H,7-8H2,1H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
IE: Ionization energy (eV).
***log*P$_{oct/wat}$**: Octanol/Water partition coefficient .
P_c: Critical Pressure (kPa).
T_{boil}: Normal Boiling Point Temperature (K).
T_c: Critical Temperature (K).
T_{fus}: Normal melting (fusion) point (K).
V_c: Critical Volume (m^3/kg-mol).