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-Methyl-Â«betaÂ»-phenethylamine
	N-Methyl-Â«betaÂ»-phenylaethylamin
	N-Methyl-Â«betaÂ»-phenylethylamine
	N-Methylbenzeneethanamine
	N-Methylphenethylamine
	N-Methylphenylethylamine
	N-Phenethylmethylamine
	NSC 113957
	Phenethylamine, N-methyl-
	WIN 5553
	«alpha»-Phenyl-«beta»-methylaminoethane
	Â«alphaÂ»-Phenyl-Â«betaÂ»-methylaminoethane
Inchi:	InChI=1S/C9H13N/c1-10-8-7-9-5-3-2-4-6-9/h2-6,10H,7-8H2,1H3
InchiKey:	SASNBVQSOZSTPD-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	CNCCc1ccccc1
Mol. weight [g/mol]:	135.21
CAS:	589-08-2

Physical Properties

Property code	Value	Unit	Source
gf	226.70	kJ/mol	Joback Method
hf	60.91	kJ/mol	Joback Method
hfus	18.21	kJ/mol	Joback Method
hvap	44.34	kJ/mol	Joback Method
ie	8.66 ± 0.20	eV	NIST Webbook
ie	8.40	eV	NIST Webbook

log10ws	-1.88		Crippen Method
logp	1.448		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
rinpol	1154.00		NIST Webbook
ripol	1571.00		NIST Webbook
ripol	1571.00		NIST Webbook
tb	476.20	K	NIST Webbook
tc	691.55	K	Joback Method
tf	270.27	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.33	J/mol×K	482.17	Joback Method
cpg	274.63	J/mol×K	517.07	Joback Method
cpg	288.10	J/mol×K	551.96	Joback Method
cpg	300.77	J/mol×K	586.86	Joback Method
cpg	312.68	J/mol×K	621.76	Joback Method
cpg	323.85	J/mol×K	656.66	Joback Method
cpg	334.34	J/mol×K	691.55	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49571e+01
Coeff. B	-4.15460e+03
Coeff. C	-7.43540e+01
Temperature range (K), min.	357.57
Temperature range (K), max.	505.08

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C589082&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

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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume