Benzeneethanamine, «beta»-methyl-

Other names:	«beta»-Methylbenzeneethanamine
	«beta»-Methylphenethylamine
	«beta»-Methylphenylethylamine
	Phenethylamine, «beta»-methyl-
	«beta»-Phenylpropylamine
	2-Phenylpropylamine
	1-Propanamine, 2-phenyl-
	Propylamine, 2-phenyl-
	1-Phenyl-1-methyl-2-amino-aethan
	1-Phenyl-1-methyl-2-aminoethane
	1-Amino-2-phenylpropane
	2-Phenyl-1-propylamine
	NSC 272273
	beta-methylphenethylamine
Inchi:	InChI=1S/C9H13N/c1-8(7-10)9-5-3-2-4-6-9/h2-6,8H,7,10H2,1H3
InchiKey:	AXORVIZLPOGIRG-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	CC(CN)c1ccccc1
Mol. weight [g/mol]:	135.21
CAS:	582-22-9

Physical Properties

Property code	Value	Unit	Source
gf	201.32	kJ/mol	Joback Method
hf	35.95	kJ/mol	Joback Method
hfus	14.78	kJ/mol	Joback Method
hvap	48.16	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.749		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpol	1129.70		NIST Webbook
tb	504.09	K	Joback Method
tc	728.62	K	Joback Method
tf	285.87	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.70	J/mol×K	504.09	Joback Method
cpg	286.20	J/mol×K	541.51	Joback Method
cpg	299.78	J/mol×K	578.93	Joback Method
cpg	312.48	J/mol×K	616.35	Joback Method
cpg	324.34	J/mol×K	653.78	Joback Method
cpg	335.40	J/mol×K	691.20	Joback Method
cpg	345.71	J/mol×K	728.62	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.20	K	1.30	NIST Webbook

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=C582229&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume