Benzeneethanamine, N,N-dimethyl-

Other names:	Benzeneethanamine, dimethyl-
	Dimethylaminoethylbenzene
	N,N-Dimethyl-2-phenethylamine
	N,N-Dimethyl-«beta»-phenethylamine
	N,N-Dimethyl-Â«betaÂ»-phenethylamine
	N,N-Dimethylbenzeneethanamine
	N,N-Dimethylphenethylamine
	N-Phenethyldimethylamine
	Phenethylamine, N,N-dimethyl-
	Phenylethylamine, N,N-dimethyl
Inchi:	InChI=1S/C10H15N/c1-11(2)9-8-10-6-4-3-5-7-10/h3-7H,8-9H2,1-2H3
InchiKey:	TXOFSCODFRHERQ-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	CN(C)CCc1ccccc1
Mol. weight [g/mol]:	149.23
CAS:	1126-71-2

Physical Properties

Property code	Value	Unit	Source
gf	256.51	kJ/mol	Joback Method
hf	54.33	kJ/mol	Joback Method
hfus	18.72	kJ/mol	Joback Method
hvap	42.17	kJ/mol	Joback Method
ie	7.70 ± 0.05	eV	NIST Webbook
ie	8.35 ± 0.14	eV	NIST Webbook
ie	7.70 ± 0.03	eV	NIST Webbook
log10ws	-1.68		Crippen Method
logp	1.791		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
rinpol	1159.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1170.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1498.00		NIST Webbook
tb	475.65 ± 5.00	K	NIST Webbook

tc	669.26	K	Joback Method
tf	261.35	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.39	J/mol×K	467.32	Joback Method
cpg	304.41	J/mol×K	500.98	Joback Method
cpg	319.51	J/mol×K	534.63	Joback Method
cpg	333.72	J/mol×K	568.29	Joback Method
cpg	347.09	J/mol×K	601.95	Joback Method
cpg	359.65	J/mol×K	635.60	Joback Method
cpg	371.44	J/mol×K	669.26	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54194e+01
Coeff. B	-4.33068e+03
Coeff. C	-7.47010e+01
Temperature range (K), min.	360.90
Temperature range (K), max.	503.14

Sources

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=C1126712&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

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