Benzeneethanamine

Other names:	(2-Aminoethyl)benzene
	(2-phenylethyl)amine
	.beta.-phenylethylamine
	1-Amino-2-phenylethane
	1-Phenyl-2-amino-athan
	1-Phenyl-2-aminoethane
	2-Amino-1-phenylethane
	2-Amino-fenylethan
	2-Fenylethylamin
	2-Phenethylamine
	2-Phenylethylamine
	2-phenylethanamine
	Ethanamine, 2-phenyl-
	Ethylamine, 2-phenyl-
	NSC 10811
	Phenethylamine
	Phenethylamine, «beta»
	Phenethylamine, Â«betaÂ»
	Phenylethylamine
	«beta»-Aminoethylbenzene
	«beta»-Phenethylamine
	«beta»-Phenylethylamine
	Â«betaÂ»-Aminoethylbenzene
	Â«betaÂ»-Phenethylamine
	Â«betaÂ»-Phenylethylamine
Inchi:	InChI=1S/C8H11N/c9-7-6-8-4-2-1-3-5-8/h1-5H,6-7,9H2
InchiKey:	BHHGXPLMPWCGHP-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	NCCc1ccccc1
Mol. weight [g/mol]:	121.18
CAS:	64-04-0

Physical Properties

Property code	Value	Unit	Source
affp	936.20	kJ/mol	NIST Webbook
basg	900.00 ± 4.00	kJ/mol	NIST Webbook

basg	902.30	kJ/mol	NIST Webbook
gf	195.34	kJ/mol	Joback Method
hf	61.87	kJ/mol	Joback Method
hfus	15.71	kJ/mol	Joback Method
hvap	56.80 ± 0.20	kJ/mol	NIST Webbook
ie	8.99 ± 0.20	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
log10ws	-1.71		Crippen Method
logp	1.188		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
rinpol	1133.00		NIST Webbook
rinpol	1100.70		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1069.90		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1133.00		NIST Webbook
ripol	1605.00		NIST Webbook
ripol	1622.00		NIST Webbook
ripol	1638.00		NIST Webbook
tb	470.70	K	NIST Webbook
tc	704.67	K	Joback Method
tf	289.60	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.62	J/mol×K	481.65	Joback Method
cpg	241.67	J/mol×K	518.82	Joback Method
cpg	253.89	J/mol×K	555.99	Joback Method
cpg	265.33	J/mol×K	593.16	Joback Method

cpg	276.02	J/mol×K	630.33	Joback Method
cpg	285.99	J/mol×K	667.50	Joback Method
cpg	295.29	J/mol×K	704.67	Joback Method
cpl	239.24	J/mol×K	298.15	NIST Webbook
hvapt	55.70 ± 0.20	kJ/mol	314.00	NIST Webbook
pvap	0.07	kPa	304.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration
pvap	0.02	kPa	287.40	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration
pvap	0.02	kPa	288.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration
pvap	0.02	kPa	288.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration

pvap	0.02	kPa	290.10	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.03	kPa	293.10	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.03	kPa	293.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.05	kPa	298.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	

pvap	0.04	kPa	298.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.04	kPa	298.30	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.05	kPa	300.10	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.06	kPa	302.00	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	

pvap	0.07	kPa	303.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.06	kPa	303.30	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.06	kPa	303.30	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.02	kPa	285.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	

pvap	0.07	kPa	305.10	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.08	kPa	305.10	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.08	kPa	306.40	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.09	kPa	308.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	

pvap	0.09	kPa	308.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.11	kPa	310.40	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.12	kPa	311.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.13	kPa	313.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	

pvap	0.13	kPa	313.40	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.14	kPa	314.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.18	kPa	317.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	
pvap	0.19	kPa	318.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration	

pvap	0.19	kPa	318.40	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration
pvap	0.22	kPa	320.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration
pvap	0.27	kPa	323.20	The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration
pvap	5.57e-03	kPa	273.26	Experimental Vapor Pressures of 2-Phenylethylamine, Benzylamine, Triethylamine, and cis-2,6-Dimethylpiperidine in the Range between 0.2 Pa and 75 kPa
pvap	0.01	kPa	283.18	Experimental Vapor Pressures of 2-Phenylethylamine, Benzylamine, Triethylamine, and cis-2,6-Dimethylpiperidine in the Range between 0.2 Pa and 75 kPa

pvap	0.03	kPa	293.12	Experimental Vapor Pressures of 2-Phenylethylamine, Benzylamine, Triethylamine, and cis-2,6-Dimethylpiperidine in the Range between 0.2 Pa and 75 kPa
pvap	0.07	kPa	303.06	Experimental Vapor Pressures of 2-Phenylethylamine, Benzylamine, Triethylamine, and cis-2,6-Dimethylpiperidine in the Range between 0.2 Pa and 75 kPa
pvap	0.13	kPa	313.07	Experimental Vapor Pressures of 2-Phenylethylamine, Benzylamine, Triethylamine, and cis-2,6-Dimethylpiperidine in the Range between 0.2 Pa and 75 kPa
pvap	0.26	kPa	323.06	Experimental Vapor Pressures of 2-Phenylethylamine, Benzylamine, Triethylamine, and cis-2,6-Dimethylpiperidine in the Range between 0.2 Pa and 75 kPa
pvap	0.48	kPa	333.11	Experimental Vapor Pressures of 2-Phenylethylamine, Benzylamine, Triethylamine, and cis-2,6-Dimethylpiperidine in the Range between 0.2 Pa and 75 kPa

pvap	0.84	kPa	343.08	Experimental Vapor Pressures of 2-Phenylethylamine, Benzylamine, Triethylamine, and cis-2,6-Dimethylpiperidine in the Range between 0.2 Pa and 75 kPa
pvap	1.33	kPa	351.79	Experimental Vapor Pressures of 2-Phenylethylamine, Benzylamine, Triethylamine, and cis-2,6-Dimethylpiperidine in the Range between 0.2 Pa and 75 kPa

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45957e+01
Coeff. B	-3.97808e+03
Coeff. C	-7.19910e+01
Temperature range (K), min.	350.02
Temperature range (K), max.	500.47

Sources

Experimental Vapor Pressures of 2-Phenylethylamine, Benzylamine, Triethylamine, and cis-2,6-Dimethylpiperidine in the Range between 0.2 Pa and 75 kPa:	https://www.doi.org/10.1021/je800603z
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Vaporization Enthalpy and Vapor Pressure of (d)-Amphetamine and of Several Primary Amines Used as Standards at T/K = 298 As Evaluated by Correlation Gas Chromatography and Transpiration:	https://www.doi.org/10.1021/je400212t
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1400.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64040&Units=SI

Legend

affp:	Proton affinity
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
hvapt:	Enthalpy of vaporization at a given temperature
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