Benzenamine, N-ethyl-

Other names:	ANILINOETHANE
	Aethylanilin
	Aniline, N-ethyl-
	ETHYLPHENYLAMINE
	Ethylaniline
	N-Ethyl-N-phenylamine
	N-Ethylaminobenzene
	N-Ethylaniline
	N-Ethylaniline
	N-Ethylbenzenamine
	NSC 8736
	UN 2272
	benzeneamine, N-ethyl-
Inchi:	InChI=1S/C8H11N/c1-2-9-8-6-4-3-5-7-8/h3-7,9H,2H2,1H3
InchiKey:	OJGMBLNIHDZDGS-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	CCNc1ccccc1
Mol. weight [g/mol]:	121.18
CAS:	103-69-5

Physical Properties

Property code	Value	Unit	Source
affp	924.80	kJ/mol	NIST Webbook
basg	892.90	kJ/mol	NIST Webbook
chg	-4714.90	kJ/mol	NIST Webbook
chl	-4724.20 ± 4.20	kJ/mol	NIST Webbook
dm	1.70	debye	KDB
gf	218.28	kJ/mol	Joback Method
hf	56.10	kJ/mol	NIST Webbook
hf	23.10	kJ/mol	NIST Webbook
hfl	4.00	kJ/mol	NIST Webbook
hfl	-29.00	kJ/mol	NIST Webbook
hfus	15.62	kJ/mol	Joback Method
hvap	52.10	kJ/mol	NIST Webbook
hvap	58.30 ± 0.60	kJ/mol	NIST Webbook
hvap	52.30	kJ/mol	NIST Webbook
ie	7.67 ± 0.06	eV	NIST Webbook

ie	7.50	eV	NIST Webbook
ie	7.56	eV	NIST Webbook
log10ws	-1.70		Aqueous Solubility Prediction Method
log10ws	-1.70		Estimated Solubility Method
logp	2.118		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=3)		KDB
pc	3708.97	kPa	Joback Method
rinpol	1111.50		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1128.00		NIST Webbook
ripol	1761.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1740.90		NIST Webbook
ripol	1751.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1761.00		NIST Webbook
ripol	1738.00		NIST Webbook
tb	479.20 ± 0.20	K	NIST Webbook
tb	477.15 ± 5.00	K	NIST Webbook
tb	478.65 ± 0.30	K	NIST Webbook
tb	476.20	K	KDB
tb	477.90	K	NIST Webbook
tb	478.65 ± 0.50	K	NIST Webbook
tb	478.15 ± 0.60	K	NIST Webbook
tb	478.65 ± 1.00	K	NIST Webbook
tb	479.70 ± 1.00	K	NIST Webbook
tb	478.65 ± 0.35	K	NIST Webbook
tc	698.00	K	KDB
tf	209.65 ± 0.40	K	NIST Webbook
tf	209.53	K	Aqueous Solubility Prediction Method
tf	209.60	K	KDB
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.49	J/mol×K	671.67	Joback Method
cpg	231.34	J/mol×K	494.69	Joback Method
cpg	243.81	J/mol×K	530.08	Joback Method
cpg	255.53	J/mol×K	565.48	Joback Method
cpg	266.53	J/mol×K	600.88	Joback Method
cpg	276.83	J/mol×K	636.28	Joback Method
cpg	218.08	J/mol×K	459.29	Joback Method
hvapt	52.20	kJ/mol	394.00	NIST Webbook
rhol	942.95	kg/m3	313.15	Comparative studies of intermolecular interaction of aromatic amines with ethyl lactate at different temperatures
rhol	947.69	kg/m3	308.15	Comparative studies of intermolecular interaction of aromatic amines with ethyl lactate at different temperatures
rhol	952.41	kg/m3	303.15	Comparative studies of intermolecular interaction of aromatic amines with ethyl lactate at different temperatures
rhol	963.00	kg/m3	293.00	KDB
rhol	938.23	kg/m3	318.15	Comparative studies of intermolecular interaction of aromatic amines with ethyl lactate at different temperatures
speedsl	1431.00	m/s	323.15	Thermodynamic and Acoustic Properties of Binary Mixtures of Ethers. 2. Diisopropyl Ether with Arylamines at (303.15, 313.15, and 323.15) K and Application of ERAS Model to Aniline Mixtures with Diisopropyl Ether and Oxolane

speedsl	1462.00	m/s	313.15	Thermodynamic and Acoustic Properties of Binary Mixtures of Ethers. 2. Diisopropyl Ether with Arylamines at (303.15, 313.15, and 323.15) K and Application of ERAS Model to Aniline Mixtures with Diisopropyl Ether and Oxolane	
speedsl	1497.00	m/s	303.15	Thermodynamic and Acoustic Properties of Binary Mixtures of Ethers. 2. Diisopropyl Ether with Arylamines at (303.15, 313.15, and 323.15) K and Application of ERAS Model to Aniline Mixtures with Diisopropyl Ether and Oxolane	
speedsl	1431.00	m/s	323.15	Thermodynamic and acoustic properties of binary mixtures of oxolane with aniline and substituted anilines at 303.15, 313.15 and 323.15 K	
speedsl	1462.00	m/s	313.15	Thermodynamic and acoustic properties of binary mixtures of oxolane with aniline and substituted anilines at 303.15, 313.15 and 323.15 K	
speedsl	1497.00	m/s	303.15	Thermodynamic and acoustic properties of binary mixtures of oxolane with aniline and substituted anilines at 303.15, 313.15 and 323.15 K	

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45550e+01
Coeff. B	-4.02911e+03
Coeff. C	-7.35200e+01
Temperature range (K), min.	355.92
Temperature range (K), max.	509.41

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.29647e+01
Coeff. B	-7.19113e+03
Coeff. C	-2.06370e+00
Coeff. D	-2.48303e-06
Temperature range (K), min.	311.15
Temperature range (K), max.	481.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Comparative studies of intermolecular interaction of aromatic amines with ethyl lactate at different temperatures:	https://www.doi.org/10.1016/j.jct.2016.09.010
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103695&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1303
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1303.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermodynamic and acoustic properties of binary mixtures of oxolane with aniline and substituted anilines at 303.15, 313.15 and 323.15 K.	https://www.doi.org/10.1016/j.tca.2010.04.025
Thermodynamic and Acoustic Properties of Binary Mixtures of Ethers. 2. Diisopropyl Ether with Arylamines at (303.15, 313.15, and 323.15) K and Application of ERAS Model to Aniline Mixtures with Diisopropyl Ether and Oxolane":	https://www.doi.org/10.1021/je1008262
Estimation of Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume