BENZENAMINE, N,N-DIETHYL-

Other names:	(Diethylamino)benzene
	DEA
	Diaethylanilin
	Diethylaniline
	Diethylphenylamine
	N,N-Diethylaminobenzene
	N,N-Diethylanilin
	N,N-Diethylbenzenamine
	N,N-diethylaniline
	N-Phenyldiethylamine
	NSC 7205
	Phenyldiethylamine
	UN 2432
	aniline, N,N-diethyl-
Inchi:	InChI=1S/C10H15N/c1-3-11(4-2)10-8-6-5-7-9-10/h5-9H,3-4H2,1-2H3
InchiKey:	GGSUCNLOZRCGPQ-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	CCN(CC)c1ccccc1
Mol. weight [g/mol]:	149.24
CAS:	91-66-7

Physical Properties

Property code	Value	Unit	Source
af	0.4292		Cheméo Relay (1.0)
affp	959.80	kJ/mol	NIST Webbook
basg	927.90	kJ/mol	NIST Webbook
chl	-6062.60	kJ/mol	NIST Webbook
chl	-6080.60 ± 2.90	kJ/mol	NIST Webbook
gf	256.51	kJ/mol	Joback Method
hf	40.00	kJ/mol	NIST Webbook
hf	62.10 ± 7.60	kJ/mol	NIST Webbook
hfl	-16.00	kJ/mol	NIST Webbook
hfl	1.80 ± 3.20	kJ/mol	NIST Webbook
hfus	18.72	kJ/mol	Joback Method
hvap	60.30	kJ/mol	NIST Webbook
hvap	56.50	kJ/mol	NIST Webbook
hvap	56.00	kJ/mol	NIST Webbook

hvap	60.30 ± 6.90	kJ/mol	NIST Webbook
ie	7.51	eV	NIST Webbook
ie	7.15	eV	NIST Webbook
ie	6.99	eV	NIST Webbook
ie	6.95 ± 0.02	eV	NIST Webbook
ie	6.98 ± 0.05	eV	NIST Webbook
ie	6.98	eV	NIST Webbook
ie	6.98 ± 0.05	eV	NIST Webbook
log10ws	-3.03		Aqueous Solubility Prediction Method
log10ws	-3.03		Estimated Solubility Method
logp	2.533		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
rinpol	1200.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1200.00		NIST Webbook
ripol	1656.00		NIST Webbook
ripol	1648.60		NIST Webbook
ripol	1659.00		NIST Webbook
ripol	1673.00		NIST Webbook
ripol	1651.00		NIST Webbook
tb	489.65 ± 0.30	K	NIST Webbook
tb	486.65 ± 1.50	K	NIST Webbook
tb	490.20 ± 0.40	K	NIST Webbook
tb	490.15 ± 0.60	K	NIST Webbook
tb	490.20 ± 0.30	K	NIST Webbook
tb	490.20 ± 0.30	K	NIST Webbook
tb	490.20 ± 0.50	K	NIST Webbook
tb	490.47 ± 0.30	K	NIST Webbook
tb	490.70 ± 1.50	K	NIST Webbook
tb	489.40 ± 1.00	K	NIST Webbook
tb	489.75 ± 0.50	K	NIST Webbook
tb	486.65 ± 5.00	K	NIST Webbook
tb	489.50	K	NIST Webbook
tc	695.85	K	Cheméo Relay (1.0)
tf	234.95	K	Aqueous Solubility Prediction Method
tf	251.85 ± 0.20	K	NIST Webbook
tf	251.85 ± 0.30	K	NIST Webbook
tf	238.75 ± 0.50	K	NIST Webbook
tf	235.10 ± 0.30	K	NIST Webbook
vc	0.500	m3/kmol	Cheméo Relay (1.0)

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
cpl	274.50	J/mol×K	302.30	NIST Webbook
cpl	274.50	J/mol×K	302.00	NIST Webbook
dvisc	0.0014020	Pa×s	313.15	Densities and Viscosities of Binary Mixtures of Propanoic Acid with N,N-Dimethylaniline and N,N-Diethylaniline at T = (303.15, 313.15, and 323.15) K
dvisc	0.0017030	Pa×s	303.15	Densities and Viscosities of Binary Mixtures of Propanoic Acid with N,N-Dimethylaniline and N,N-Diethylaniline at T = (303.15, 313.15, and 323.15) K
dvisc	0.0010487	Pa×s	323.15	Densities and Viscosities of Binary Mixtures of Propanoic Acid with N,N-Dimethylaniline and N,N-Diethylaniline at T = (303.15, 313.15, and 323.15) K
hvapt	46.32	kJ/mol	488.20	NIST Webbook
hvapt	54.50	kJ/mol	418.00	NIST Webbook

rhol	913.80	kg/m3	318.15	Studies on the importance of chain length of alkanols on the thermodynamic and transport properties of liquid mixtures at various temperatures	
rhol	917.90	kg/m3	313.15	Volumetric and transport properties of binary liquid mixtures of sulfolane with aniline, N,N-dimethylaniline and N,N-diethylaniline at different temperatures and atmospheric pressure	
rhol	925.80	kg/m3	303.15	Studies on the importance of chain length of alkanols on the thermodynamic and transport properties of liquid mixtures at various temperatures	
rhol	921.90	kg/m3	308.15	Volumetric and transport properties of binary liquid mixtures of sulfolane with aniline, N,N-dimethylaniline and N,N-diethylaniline at different temperatures and atmospheric pressure	
rhol	925.90	kg/m3	303.15	Volumetric and transport properties of binary liquid mixtures of sulfolane with aniline, N,N-dimethylaniline and N,N-diethylaniline at different temperatures and atmospheric pressure	

rhol	917.90	kg/m3	313.15	Studies on the importance of chain length of alkanols on the thermodynamic and transport properties of liquid mixtures at various temperatures
rhol	921.80	kg/m3	308.15	Studies on the importance of chain length of alkanols on the thermodynamic and transport properties of liquid mixtures at various temperatures
speedsl	1396.00	m/s	313.15	Thermodynamic and acoustic properties of binary mixtures of ethers. IV. Diisopropyl ether or oxolane with N,N-dimethylaniline or N,Ndiethylaniline at 303.15, 313.15 and 323.15 K
speedsl	1358.00	m/s	323.15	Thermodynamic and acoustic properties of binary mixtures of ethers. IV. Diisopropyl ether or oxolane with N,N-dimethylaniline or N,Ndiethylaniline at 303.15, 313.15 and 323.15 K
speedsl	1434.00	m/s	303.15	Thermodynamic and acoustic properties of binary mixtures of ethers. IV. Diisopropyl ether or oxolane with N,N-dimethylaniline or N,Ndiethylaniline at 303.15, 313.15 and 323.15 K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.06064e+01
Coeff. B	-9.72540e+03
Coeff. C	-9.15681e+00
Coeff. D	2.48168e-06
Temperature range (K), min.	235.15
Temperature range (K), max.	702.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0, beta):	
Volumetric and transport properties of binary liquid mixtures of sulfolane with aniline, N,N-dimethylaniline and N,N-diethylaniline at different temperatures and atmospheric pressure:	https://www.doi.org/10.1016/j.jct.2015.12.030
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Thermodynamic and acoustic properties of binary mixtures of ethers. IV. Diisopropyl ether or oxolane with N,N-dimethylaniline or N,N-diethylaniline at 303.15, 313.15 and 323.15 K:	https://www.doi.org/10.1016/j.tca.2011.02.004
Cheméo Relay (1.0):	
Studies on the importance of chain length of alkanols on the thermodynamic and transport properties of liquid mixtures at various temperatures:	https://www.doi.org/10.1016/j.jct.2016.12.019
Physical Properties and Viscosities of Binary Mixtures of Propanoic Acid with N,N-Dimethylaniline and N,N-Diethylaniline at T = (303.15, 313.15, and 323.15) K:	https://www.doi.org/10.1021/je200862b
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1312.mol
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1312
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91667&Units=SI

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
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
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