Benzenamine, 2,6-diethyl-

Other names:	2,6-DIETHYLBENZENAMINE
	2,6-Diethylaniline
	2,6-diethylaniline (DEA)
	Aniline, 2,6-diethyl-
Inchi:	InChI=1S/C10H15N/c1-3-8-6-5-7-9(4-2)10(8)11/h5-7H,3-4,11H2,1-2H3
InchiKey:	FOYHNROGBXVLLX-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	CCc1cccc(CC)c1N
Mol. weight [g/mol]:	149.23
CAS:	579-66-8

Physical Properties

Property code	Value	Unit	Source
gf	192.92	kJ/mol	Joback Method
hf	-2.35	kJ/mol	Joback Method
hfus	20.12	kJ/mol	Joback Method
hvap	65.90 ± 0.60	kJ/mol	NIST Webbook
ie	7.77	eV	NIST Webbook
log10ws	-2.35		Aqueous Solubility Prediction Method
logp	2.394		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
rinpol	227.43		NIST Webbook
rinpol	1295.60		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	227.43		NIST Webbook
tb	537.37	K	Joback Method
tc	755.40	K	Joback Method
tf	276.65	K	Aqueous Solubility Prediction Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.09	J/mol×K	537.37	Joback Method
cpg	330.39	J/mol×K	573.71	Joback Method
cpg	343.90	J/mol×K	610.05	Joback Method
cpg	356.65	J/mol×K	646.38	Joback Method
cpg	368.66	J/mol×K	682.72	Joback Method
cpg	379.98	J/mol×K	719.06	Joback Method
cpg	390.61	J/mol×K	755.40	Joback Method
hvapt	69.50 ± 0.60	kJ/mol	306.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44406e+01
Coeff. B	-4.23692e+03
Coeff. C	-8.25550e+01
Temperature range (K), min.	381.92
Temperature range (K), max.	546.66

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.46372e+02
Coeff. B	-1.50264e+04
Coeff. C	-1.82753e+01
Coeff. D	6.43473e-06
Temperature range (K), min.	276.65
Temperature range (K), max.	678.00

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1313
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1313.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C579668&Units=SI

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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume