Benzenamine, N-butyl-

Other names:	4-(PHENYLAMINO)BUTANE
	Aniline, N-butyl-
	N-(n-Butyl)aniline
	N-BUTYL BENZENAMINE
	N-Butylaniline
	N-Butylbenzenamine
	NSC 7114
	UN 2738
Inchi:	InChI=1S/C10H15N/c1-2-3-9-11-10-7-5-4-6-8-10/h4-8,11H,2-3,9H2,1H3
InchiKey:	VSHTWPWTCXQLQN-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	CCCCNc1ccccc1
Mol. weight [g/mol]:	149.23
CAS:	1126-78-9

Physical Properties

Property code	Value	Unit	Source
gf	235.12	kJ/mol	Joback Method
hf	40.27	kJ/mol	Joback Method
hfus	20.80	kJ/mol	Joback Method
hvap	46.57	kJ/mol	Joback Method
ie	7.53	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
log10ws	-2.74		Crippen Method
logp	2.899		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	2830.00	kPa	KDB
rinpol	1300.00		NIST Webbook
rinpol	1300.00		NIST Webbook
ripol	1893.00		NIST Webbook
ripol	1893.00		NIST Webbook
tb	513.90	K	KDB
tb	512.20	K	NIST Webbook
tb	510.65 ± 1.50	K	NIST Webbook
tc	721.00	K	KDB
tf	259.00	K	KDB
tf	258.10 ± 0.60	K	NIST Webbook

vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.27	J/mol×K	642.61	Joback Method
cpg	372.21	J/mol×K	677.00	Joback Method
cpg	304.53	J/mol×K	505.05	Joback Method
cpg	319.73	J/mol×K	539.44	Joback Method
cpg	334.07	J/mol×K	573.83	Joback Method
cpg	347.57	J/mol×K	608.22	Joback Method
cpg	383.43	J/mol×K	711.40	Joback Method
hvapt	55.60	kJ/mol	528.00	NIST Webbook
rhol	932.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52470e+01
Coeff. B	-4.54080e+03
Coeff. C	-8.47790e+01
Temperature range (K), min.	388.32
Temperature range (K), max.	541.80

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.38834e+02
Coeff. B	-1.31509e+04
Coeff. C	-1.77347e+01
Coeff. D	7.85494e-06
Temperature range (K), min.	385.00
Temperature range (K), max.	560.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1311.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1126789&Units=SI
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=1311
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rhol:	Liquid Density
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