

Benzenamine, 4-butyl-

Other names:	1-Amino-4-butylbenzene 4-Butylaniline 4-Butylbenzenamine 4-Butylbenzeneamine 4-n-Butylaniline Aniline, 4-butyl- Aniline, p-butyl- p-Aminobutylbenzene p-Butyl aniline p-Butylaminobenzene p-n-Butylaniline
Inchi:	InChI=1S/C10H15N/c1-2-3-4-9-5-7-10(11)8-6-9/h5-8H,2-4,11H2,1H3
InchiKey:	OGIQUQKNJTLSZ-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	CCCCc1ccc(N)cc1
Mol. weight [g/mol]:	149.23
CAS:	104-13-2

Physical Properties

Property code	Value	Unit	Source
gf	202.55	kJ/mol	Joback Method
hf	9.12	kJ/mol	Joback Method
hfus	20.51	kJ/mol	Joback Method
hvap	51.43	kJ/mol	Joback Method
ie	7.60 ± 0.10	eV	NIST Webbook
log10ws	-2.75		Crippen Method
logp	2.611		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
ripol	2155.00		NIST Webbook
tb	532.39	K	Joback Method
tc	749.29	K	Joback Method
tf	324.66	K	Joback Method
vc	0.516	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.19	J/mol×K	532.39	Joback Method
cpg	330.82	J/mol×K	568.54	Joback Method
cpg	344.61	J/mol×K	604.69	Joback Method
cpg	357.59	J/mol×K	640.84	Joback Method
cpg	369.79	J/mol×K	676.99	Joback Method
cpg	381.24	J/mol×K	713.14	Joback Method
cpg	391.97	J/mol×K	749.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	392.20	K	2.00	NIST Webbook
tbrp	406.70	K	1.90	NIST Webbook
tbrp	399.00	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53750e+01
Coeff. B	-4.60602e+03
Coeff. C	-8.57100e+01
Temperature range (K), min.	391.00
Temperature range (K), max.	543.41

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C104132&Units=SI>

The Yaws Handbook of Vapor Pressure:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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
ripol:	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

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