Benzenebutanamine

Other names:	1-Amino-4-phenylbutane
	4-Amino-1-phenylbutane
	4-Phenylbutylamine
	4-Phenylbutylamine-1
	Butylamine, 4-phenyl-
Inchi:	InChI=1S/C10H15N/c11-9-5-4-8-10-6-2-1-3-7-10/h1-3,6-7H,4-5,8-9,11H2
InchiKey:	AGNFWIZBEATIAK-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	NCCCCc1ccccc1
Mol. weight [g/mol]:	149.23
CAS:	13214-66-9

Physical Properties

Property code	Value	Unit	Source
basg	925.00 ± 12.00	kJ/mol	NIST Webbook
gf	212.18	kJ/mol	Joback Method
hf	20.59	kJ/mol	Joback Method
hfus	20.89	kJ/mol	Joback Method
hvap	50.77	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	1.968		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpol	1285.10		NIST Webbook
rinpol	1285.10		NIST Webbook
tb	527.41	K	Joback Method
tc	743.16	K	Joback Method
tf	312.14	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.18	J/mol×K	527.41	Joback Method

cpg	331.17	J/mol×K	563.37	Joback Method
cpg	345.25	J/mol×K	599.33	Joback Method
cpg	358.46	J/mol×K	635.29	Joback Method
cpg	370.85	J/mol×K	671.25	Joback Method
cpg	382.45	J/mol×K	707.21	Joback Method
cpg	393.30	J/mol×K	743.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	396.70	K	2.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44981e+01
Coeff. B	-4.17685e+03
Coeff. C	-8.07150e+01
Temperature range (K), min.	374.64
Temperature range (K), max.	535.38

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13214669&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/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

basg:	Gas basicity
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
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