Benzenamine, N-(1-methylethyl)-

Other names:	Aniline, N-isopropyl-
	Isopropylaniline
	N-(1-Methylethyl)benzenamine
	N-(1-Methylethyl)phenylamine
	N-Isopropyl-N-phenylamine
	N-Isopropylaniline
	N-Isopropylbenzenamine
	N-Phenylisopropylamine
	Phenylisopropylamine
Inchi:	InChI=1S/C9H13N/c1-8(2)10-9-6-4-3-5-7-9/h3-8,10H,1-2H3
InchiKey:	FRCFWPVMFJMNDP-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	CC(C)Nc1ccccc1
Mol. weight [g/mol]:	135.21
CAS:	768-52-5

Physical Properties

Property code	Value	Unit	Source
gf	224.26	kJ/mol	Joback Method
hf	55.63	kJ/mol	Joback Method
hfus	14.68	kJ/mol	Joback Method
hvap	43.95	kJ/mol	Joback Method
ie	7.50	eV	NIST Webbook
log10ws	-2.43		Crippen Method
logp	2.507		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
rinpol	1127.20		NIST Webbook
tb	481.73	K	Joback Method
tc	696.01	K	Joback Method
tf	255.27	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.51	J/mol×K	481.73	Joback Method
cpg	275.23	J/mol×K	517.44	Joback Method
cpg	289.07	J/mol×K	553.16	Joback Method
cpg	302.07	J/mol×K	588.87	Joback Method
cpg	314.25	J/mol×K	624.59	Joback Method
cpg	325.67	J/mol×K	660.30	Joback Method
cpg	336.35	J/mol×K	696.01	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.50 ± 0.50	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.30590e+01
Coeff. B	-3.60663e+03
Coeff. C	-7.35200e+01
Temperature range (K), min.	355.92
Temperature range (K), max.	539.04

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C768525&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

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
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