Benzenamine, 2-(1-methylethyl)-

Other names:	1-Amino-2-isopropylbenzene
	2-(1-Methylethyl)benzenamine
	2-Aminoisopropylbenzene
	2-Isopropylaniline
	Aniline, o-isopropyl-
	o-Aminocumene
	o-Aminoisopropylbenzene
	o-Cumidine
	o-Isopropylaniline
Inchi:	InChI=1S/C9H13N/c1-7(2)8-5-3-4-6-9(8)10/h3-7H,10H2,1-2H3
InchiKey:	YKOLZVXSPGIIBJ-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	CC(C)c1ccccc1N
Mol. weight [g/mol]:	135.21
CAS:	643-28-7

Physical Properties

Property code	Value	Unit	Source
gf	191.69	kJ/mol	Joback Method
hf	24.48	kJ/mol	Joback Method
hfus	14.39	kJ/mol	Joback Method
hvap	61.80 ± 0.90	kJ/mol	NIST Webbook
log10ws	-2.29		Crippen Method
logp	2.392		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
tb	509.07	K	Joback Method
tc	734.84	K	Joback Method
tf	298.39	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	271.79	J/mol×K	509.07	Joback Method
cpg	285.89	J/mol×K	546.70	Joback Method
cpg	299.13	J/mol×K	584.33	Joback Method
cpg	311.56	J/mol×K	621.96	Joback Method
cpg	323.20	J/mol×K	659.58	Joback Method
cpg	334.09	J/mol×K	697.21	Joback Method
cpg	344.26	J/mol×K	734.84	Joback Method
hvapt	61.30 ± 0.90	kJ/mol	306.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	385.70	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43022e+01
Coeff. B	-4.08941e+03
Coeff. C	-7.85240e+01
Temperature range (K), min.	370.32
Temperature range (K), max.	533.37

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C643287&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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
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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