N-Isopropylcyclohexylamine

Other names:	Cyclohexanamine, N-(1-methylethyl)-
	Cyclohexylamine, N-isopropyl-
	Cyclohexylisopropylamine
	N-Cyclohexylisopropylamine
Inchi:	InChI=1S/C9H19N/c1-8(2)10-9-6-4-3-5-7-9/h8-10H,3-7H2,1-2H3
InchiKey:	UYYCVBASZNFFRX-UHFFFAOYSA-N
Formula:	C9H19N
SMILES:	CC(C)NC1CCCCC1
Mol. weight [g/mol]:	141.25
CAS:	1195-42-2

Physical Properties

Property code	Value	Unit	Source
gf	136.30	kJ/mol	Joback Method
hf	-126.58	kJ/mol	Joback Method
hfus	12.48	kJ/mol	Joback Method
hvap	42.11	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.317		Crippen Method
mcvol	136.790	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
rinpol	1022.00		NIST Webbook
tb	474.60	K	Joback Method
tc	680.97	K	Joback Method
tf	236.23	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.24	J/mol×K	474.60	Joback Method
cpg	327.44	J/mol×K	508.99	Joback Method
cpg	345.64	J/mol×K	543.39	Joback Method
cpg	362.86	J/mol×K	577.78	Joback Method

cpg	379.14	J/mol×K	612.18	Joback Method
cpg	394.51	J/mol×K	646.57	Joback Method
cpg	409.00	J/mol×K	680.97	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	335.70	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.29778e+01
Coeff. B	-3.32506e+03
Coeff. C	-6.37300e+01
Temperature range (K), min.	325.75
Temperature range (K), max.	497.45

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=C1195422&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

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