1-Propanamine, N-(1-methylethyl)-

Other names:	N-isopropylpropylamine
	Propylisopropylamine
	isopropy-n-propylamine
Inchi:	InChI=1S/C6H15N/c1-4-5-7-6(2)3/h6-7H,4-5H2,1-3H3
InchiKey:	VLSTXUUYLIALPB-UHFFFAOYSA-N
Formula:	C6H15N
SMILES:	CCCNC(C)C
Mol. weight [g/mol]:	101.19
CAS:	21968-17-2

Physical Properties

Property code	Value	Unit	Source
gf	86.59	kJ/mol	Joback Method
hf	-118.98	kJ/mol	Joback Method
hfus	12.87	kJ/mol	Joback Method
hvap	37.30 ± 0.10	kJ/mol	NIST Webbook
log10ws	-1.64		Crippen Method
logp	1.394		Crippen Method
mcvol	105.380	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
rinpol	694.00		NIST Webbook
tb	369.65 ± 3.00	K	NIST Webbook
tc	560.25	K	Joback Method
tf	195.04	K	Joback Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.15	J/mol×K	386.41	Joback Method
cpg	210.90	J/mol×K	415.38	Joback Method
cpg	222.20	J/mol×K	444.36	Joback Method
cpg	233.07	J/mol×K	473.33	Joback Method
cpg	243.51	J/mol×K	502.30	Joback Method

cpg	253.53	J/mol×K	531.27	Joback Method
cpg	263.15	J/mol×K	560.25	Joback Method
hvapt	36.20 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	35.20 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	34.10 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	33.00 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	36.20	kJ/mol	340.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41714e+01
Coeff. B	-2.72333e+03
Coeff. C	-8.45770e+01
Temperature range (K), min.	280.73
Temperature range (K), max.	391.95

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21968172&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume