1,3-Propanediamine, N-(1-methylethyl)-

Other names:	1,3-Propanediamine, N-isopropyl-
	N-Isopropyl-1,3-propanediamine
	N-Isopropyl-1,3-propylenediamine
	N-Isopropyltrimethylenediamine
	N-isopropylpropane-1,3-diamine
Inchi:	InChI=1S/C6H16N2/c1-6(2)8-5-3-4-7/h6,8H,3-5,7H2,1-2H3
InchiKey:	KFDIDIIKNMZLRZ-UHFFFAOYSA-N
Formula:	C6H16N2
SMILES:	CC(C)NCCCN
Mol. weight [g/mol]:	116.20
CAS:	3360-16-5

Physical Properties

Property code	Value	Unit	Source
gf	153.04	kJ/mol	Joback Method
hf	-85.19	kJ/mol	Joback Method
hfus	18.07	kJ/mol	Joback Method
hvap	45.64	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	0.333		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
tb	435.20	K	NIST Webbook
tc	646.74	K	Joback Method
tf	278.30	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.54	J/mol×K	458.94	Joback Method
cpg	266.91	J/mol×K	490.24	Joback Method
cpg	278.73	J/mol×K	521.54	Joback Method
cpg	290.02	J/mol×K	552.84	Joback Method

cpg	300.80	J/mol×K	584.14	Joback Method
cpg	311.08	J/mol×K	615.44	Joback Method
cpg	320.87	J/mol×K	646.74	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56635e+01
Coeff. B	-4.12072e+03
Coeff. C	-6.21220e+01
Temperature range (K), min.	330.12
Temperature range (K), max.	460.18

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3360165&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume