1-Propanamine, N,2-dimethyl-

Other names:	2-Methyl-1-(methylamino)propane
	Isobutylmethylamine
	Methylisobutylamine
	N,2-Dimethylpropylamine
	N-Isobutylmethylamine
	N-Methylisobutylamine
	Propylamine, N,2-dimethyl-
Inchi:	InChI=1S/C5H13N/c1-5(2)4-6-3/h5-6H,4H2,1-3H3
InchiKey:	QKYWADPCTHTJHQ-UHFFFAOYSA-N
Formula:	C5H13N
SMILES:	CNCC(C)C
Mol. weight [g/mol]:	87.16
CAS:	625-43-4

Physical Properties

Property code	Value	Unit	Source
gf	78.17	kJ/mol	Joback Method
hf	-98.34	kJ/mol	Joback Method
hfus	10.28	kJ/mol	Joback Method
hvap	32.77	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	0.862		Crippen Method
mcvol	91.290	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
rinpol	635.00		NIST Webbook
rinpol	635.00		NIST Webbook
ripol	803.00		NIST Webbook
tb	363.53	K	Joback Method
tc	537.86	K	Joback Method
tf	183.77	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.53	J/mol×K	363.53	Joback Method
cpg	172.97	J/mol×K	392.59	Joback Method
cpg	183.01	J/mol×K	421.64	Joback Method
cpg	192.67	J/mol×K	450.70	Joback Method
cpg	201.96	J/mol×K	479.75	Joback Method
cpg	210.89	J/mol×K	508.81	Joback Method
cpg	219.45	J/mol×K	537.86	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43455e+01
Coeff. B	-2.59238e+03
Coeff. C	-8.01390e+01
Temperature range (K), min.	264.55
Temperature range (K), max.	367.10

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C625434&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume