Diisopropylamine

Other names:	(iso-C3H7)2NH
	2-Propanamine, N-(1-methylethyl)-
	Bis(isopropyl)amine
	N,N-Diisopropylamine
	N-(1-Methylethyl)-2-propamine
	N-(1-Methylethyl)-2-propanamine
	N-Isopropyl-1-amino-2-methylethane
	N-isopropyl-isopropylamine
	NSC 6758
	UN 1158
Inchi:	InChI=1S/C6H15N/c1-5(2)7-6(3)4/h5-7H,1-4H3
InchiKey:	UAOMVDZJSHZZME-UHFFFAOYSA-N
Formula:	C6H15N
SMILES:	CC(C)NC(C)C
Mol. weight [g/mol]:	101.19
CAS:	108-18-9

Physical Properties

Property code	Value	Unit	Source
affp	971.90	kJ/mol	NIST Webbook
basg	938.60	kJ/mol	NIST Webbook
chl	-4333.80 ± 2.50	kJ/mol	NIST Webbook
chl	-4326.30 ± 0.42	kJ/mol	NIST Webbook
gf	84.15	kJ/mol	Joback Method
hf	-143.70	kJ/mol	NIST Webbook
hf	-136.30 ± 2.60	kJ/mol	NIST Webbook
hfl	-171.00 ± 2.60	kJ/mol	NIST Webbook
hfl	-178.40 ± 0.04	kJ/mol	NIST Webbook
hfus	9.35	kJ/mol	Joback Method
hvap	34.60 ± 0.10	kJ/mol	NIST Webbook
hvap	33.80 ± 0.20	kJ/mol	NIST Webbook
hvap	34.50 ± 0.10	kJ/mol	NIST Webbook
hvap	34.51 ± 0.08	kJ/mol	NIST Webbook
hvap	34.60	kJ/mol	NIST Webbook
hvap	34.70	kJ/mol	NIST Webbook
hvap	34.72	kJ/mol	NIST Webbook
ie	7.73 ± 0.03	eV	NIST Webbook

ie	7.60 ± 0.10	eV	NIST Webbook
log10ws	-1.75		Crippen Method
logp	1.393		Crippen Method
mcvol	105.380	ml/mol	McGowan Method
pc	3020.00 ± 30.17	kPa	NIST Webbook
rinpol	619.00		NIST Webbook
rinpol	644.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	644.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	655.00		NIST Webbook
rinpol	622.00		NIST Webbook
rinpol	641.00		NIST Webbook
ripol	752.00		NIST Webbook
ripol	752.00		NIST Webbook
ripol	740.00		NIST Webbook
ripol	762.00		NIST Webbook
ripol	762.00		NIST Webbook
ripol	740.00		NIST Webbook
ripol	756.00		NIST Webbook
ripol	760.00		NIST Webbook
tb	357.15 ± 4.00	K	NIST Webbook
tb	355.40 ± 3.00	K	NIST Webbook
tb	357.15 ± 2.00	K	NIST Webbook
tb	357.15 ± 4.00	K	NIST Webbook
tb	357.15 ± 3.00	K	NIST Webbook
tb	357.00 ± 3.00	K	NIST Webbook
tb	355.15 ± 3.00	K	NIST Webbook
tb	357.10	K	NIST Webbook
tb	357.00 ± 0.30	K	NIST Webbook
tb	357.05	K	NIST Webbook
tb	356.45 ± 0.30	K	NIST Webbook
tb	356.90 ± 2.00	K	NIST Webbook
tb	357.05 ± 2.00	K	NIST Webbook
tb	357.20	K	NIST Webbook
tb	357.15 ± 3.00	K	NIST Webbook
tc	523.10 ± 0.52	K	NIST Webbook
tc	522.20	K	NIST Webbook
tf	212.15 ± 1.00	K	NIST Webbook
tf	176.85	K	NIST Webbook
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.06	J/mol×K	385.97	Joback Method
cpg	211.19	J/mol×K	415.63	Joback Method
cpg	222.83	J/mol×K	445.28	Joback Method
cpg	234.02	J/mol×K	474.94	Joback Method
cpg	244.75	J/mol×K	504.60	Joback Method
cpg	255.03	J/mol×K	534.25	Joback Method
cpg	264.88	J/mol×K	563.91	Joback Method
hvapt	35.40	kJ/mol	336.00	NIST Webbook
hvapt	30.40	kJ/mol	357.10	NIST Webbook
hvapt	35.60	kJ/mol	320.00	NIST Webbook
hvapt	33.70 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	32.60 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	31.50 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	30.20 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	34.40	kJ/mol	328.00	NIST Webbook
hvapt	34.00	kJ/mol	291.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.95430e+02
Coeff. B	-1.50323e+04
Coeff. C	-4.32974e+01
Coeff. D	4.55601e-05
Temperature range (K), min.	176.85
Temperature range (K), max.	523.10

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C108189&Units=SI

KDB Pure (Korean Thermophysical Properties Databank): https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1271

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1271
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1271.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
ie:	Ionization energy
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