Diisopropylamine

Other names:	2-propanamine, N-isopropyl-
	DIPA
	N-ISOPROPYL-1-AMINO-2-METHYLETHANE
	N-isopropyl-1-methylethanamine
	N-isopropyl-2-propanamine
	bis(1-methylethyl)amine
Inchi:	InChI=1S/C6H15NO2/c1-5(8)3-7-4-6(2)9/h5-9H,3-4H2,1-2H3
InchiKey:	LVTYICIALWPMFW-UHFFFAOYSA-N
Formula:	C6H15NO2
SMILES:	CC(O)CNCC(C)O
Mol. weight [g/mol]:	133.19
CAS:	108-18-9

Physical Properties

Property code	Value	Unit	Source
af	0.3600		KDB
dm	1.00	debye	KDB
gf	-189.49	kJ/mol	Joback Method
hf	-428.72	kJ/mol	Joback Method
hfus	22.74	kJ/mol	Thermodynamics of aqueous solutions of methyldiethanolamine and diisopropanolamine.
hvap	67.97	kJ/mol	Joback Method
log10ws	-0.27		Crippen Method
logp	-0.662		Crippen Method
mcvol	117.120	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=3)		KDB
pc	3020.00	kPa	KDB
tb	357.00	K	KDB
tc	523.10	K	KDB
tf	212.00	K	KDB
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.16	J/mol×K	570.33	Joback Method
cpg	309.37	J/mol×K	598.03	Joback Method
cpg	318.18	J/mol×K	625.72	Joback Method
cpg	326.61	J/mol×K	653.42	Joback Method
cpg	334.66	J/mol×K	681.12	Joback Method
cpg	342.35	J/mol×K	708.81	Joback Method
cpg	349.69	J/mol×K	736.51	Joback Method
rfi	1.39220		293.15	Measurement and correlation of the mutual solubility of diisopropylamine + water and triethylamine + water systems at high pressure
rfi	1.39240		293.15	Vapor-Liquid Equilibrium and Excess Gibbs Energies of Hexane + N,N-Dimethyl Formamide, 2-Methylpropan-2-ol + 2-Aminophenol, N,N-Dimethyl Formamide, and 2-Propanol + Diisopropyl Amine at 94.4 kPa
rhol	712.44	kg/m3	298.15	Acoustic, volumetric and spectral studies of binary liquid mixtures of aliphatic dialkylamine and 2-alkanols at different temperatures
rhol	717.30	kg/m3	293.15	Acoustic, volumetric and spectral studies of binary liquid mixtures of aliphatic dialkylamine and 2-alkanols at different temperatures
rhol	722.00	kg/m3	295.00	KDB

rhol	707.55	kg/m3	303.15	Acoustic, volumetric and spectral studies of binary liquid mixtures of aliphatic dialkylamine and 2-alkanols at different temperatures
rhol	702.66	kg/m3	308.15	Acoustic, volumetric and spectral studies of binary liquid mixtures of aliphatic dialkylamine and 2-alkanols at different temperatures
rhol	720.89	kg/m3	293.15	Excess molar volumes of Diisopropylamine + (C1-C5) Alkan-1-ols: application of the ERAS model and cubic EOS
rhol	715.35	kg/m3	298.15	Excess molar volumes of Diisopropylamine + (C1-C5) Alkan-1-ols: application of the ERAS model and cubic EOS
rhol	710.23	kg/m3	303.15	Excess molar volumes of Diisopropylamine + (C1-C5) Alkan-1-ols: application of the ERAS model and cubic EOS
rhol	699.71	kg/m3	313.15	Excess molar volumes of Diisopropylamine + (C1-C5) Alkan-1-ols: application of the ERAS model and cubic EOS
rhol	716.37	kg/m3	293.15	Density, Speed of Sound, Viscosity, Excess Properties, and Prigogine Flory Patterson (PFP) Theory of Binary Mixtures of Amine and Alcohols

rhol	711.51	kg/m3	298.15	Density, Speed of Sound, Viscosity, Excess Properties, and Prigogine Flory Patterson (PFP) Theory of Binary Mixtures of Amine and Alcohols	
rhol	706.63	kg/m3	303.15	Density, Speed of Sound, Viscosity, Excess Properties, and Prigogine Flory Patterson (PFP) Theory of Binary Mixtures of Amine and Alcohols	
rhol	701.74	kg/m3	308.15	Density, Speed of Sound, Viscosity, Excess Properties, and Prigogine Flory Patterson (PFP) Theory of Binary Mixtures of Amine and Alcohols	
rhol	696.81	kg/m3	313.15	Density, Speed of Sound, Viscosity, Excess Properties, and Prigogine Flory Patterson (PFP) Theory of Binary Mixtures of Amine and Alcohols	

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48638e+01
Coeff. B	-3.32495e+03
Coeff. C	-3.24720e+01
Temperature range (K), min.	260.58
Temperature range (K), max.	380.55

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002369&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Excess molar volumes of Diisopropylamine + (C1-C5) Alkan-1-ols: application of the ERAS model and cubic EOS:	https://www.doi.org/10.1016/j.tca.2011.05.006
Measurement and correlation of the mutual solubility of diisopropylamine + water and triethylamine + water systems at high pressure.:	https://www.doi.org/10.1016/j.fluid.2013.11.027
Vapor-Liquid Equilibrium and Excess Gibbs Energies of Hexane + N,N-Dimethyl Formamide, 2-Methylpropan-2-ol + N,N-Dimethyl Formamide, and 2-Propanol + Diisopropyl Amine at 94.4 kPa:	https://www.doi.org/10.1021/je7001336
Acoustic, volumetric and spectral studies of binary liquid mixtures of diisopropylamine and 2-alkanols at different temperatures:	https://www.doi.org/10.1016/j.jct.2018.12.012
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1271
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Density, Speed of Sound, Viscosity, Excess Properties, and Prigogine Flory Patterson (PFP) Theory of Binary Mixtures of Amine and Alcohols:	https://www.doi.org/10.1021/acs.jced.5b00216
Thermodynamics of aqueous solutions of methyldiethanolamine and diisopropanolamine.:	https://www.doi.org/10.1016/j.fluid.2010.08.026

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume