

1-Octanamine, N,N-dioctyl-

Other names:	336S Alamine 308 Alamine 336 Alamine 3365 Alamine 336S Farmin 08 N,N-dioctyl-1-octanamine NSC 11034 TOA Tri-N-caprylylamine Tri-n-octylamine Tricaprylamine Tricaprylylamine Trioctylamine
Inchi:	InChI=1S/C24H51N/c1-4-7-10-13-16-19-22-25(23-20-17-14-11-8-5-2)24-21-18-15-12-9-6
InchiKey:	XTAZYLNFDRKIHJ-UHFFFAOYSA-N
Formula:	C24H51N
SMILES:	CCCCCCCCN(CCCCCCCC)CCCCCCCC
Mol. weight [g/mol]:	353.67
CAS:	1116-76-3

Physical Properties

Property code	Value	Unit	Source
chl	-16147.90 ± 2.10	kJ/mol	NIST Webbook
chl	-16145.40 ± 3.60	kJ/mol	NIST Webbook
gf	261.98	kJ/mol	Joback Method
hf	-474.80	kJ/mol	NIST Webbook
hf	-477.00 ± 15.00	kJ/mol	NIST Webbook
hfl	-585.30 ± 2.10	kJ/mol	NIST Webbook
hfl	-587.50 ± 3.80	kJ/mol	NIST Webbook
hfus	60.94	kJ/mol	Joback Method
hvap	110.50	kJ/mol	NIST Webbook
hvap	110.40 ± 1.50	kJ/mol	NIST Webbook
hvap	110.00 ± 15.00	kJ/mol	NIST Webbook
log10ws	-8.44		Crippen Method
logp	8.370		Crippen Method
mcvol	359.000	ml/mol	McGowan Method

pc	805.25	kPa	Joback Method
rinpol	2297.00		NIST Webbook
rinpol	2297.00		NIST Webbook
rinpol	2297.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2290.00		NIST Webbook
tb	630.15 ± 4.00	K	NIST Webbook
tb	639.20	K	NIST Webbook
tc	932.42	K	Joback Method
tf	238.55 ± 1.00	K	NIST Webbook
tf	238.73	K	Solid-Liquid Equilibria, Excess Molar Volumes, and Molar Refractivity Deviations for Extractive Solvents of Molybdenum
vc	1.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1132.54	J/mol×K	760.96	Joback Method
cpg	1177.65	J/mol×K	818.11	Joback Method
cpg	1155.63	J/mol×K	789.54	Joback Method
cpg	1255.89	J/mol×K	932.42	Joback Method
cpg	1237.72	J/mol×K	903.85	Joback Method
cpg	1218.65	J/mol×K	875.27	Joback Method
cpg	1198.64	J/mol×K	846.69	Joback Method
cpl	750.80	J/mol×K	298.15	NIST Webbook
hvapt	100.10	kJ/mol	298.00	Evaluation of the Vaporization Enthalpies and Liquid Vapor Pressures of (R)-Deprenyl, (S)-Benzphetamine, Alverine, and a Series of Aliphatic Tertiary Amines by Correlation Gas Chromatography at T/K = 298.15
hvapt	70.60	kJ/mol	603.50	NIST Webbook

hvapt	71.85	kJ/mol	505.00	Thermodynamics and kinetics analysis of thermal dissociation of tri-n-octylamine hydrochloride in open system: A DFT and TGA study
rhol	803.88	kg/m3	303.15	Density, viscosity and excess molar volume of binary mixtures of tri-n-octylamine + diluents (n-heptane, n-octane, n-nonane, and n-decane) at various temperatures
rhol	810.48	kg/m3	293.15	Density, viscosity and excess molar volume of binary mixtures of tri-n-octylamine + diluents (n-heptane, n-octane, n-nonane, and n-decane) at various temperatures
rhol	817.08	kg/m3	283.15	Density, viscosity and excess molar volume of binary mixtures of tri-n-octylamine + diluents (n-heptane, n-octane, n-nonane, and n-decane) at various temperatures
rhol	810.03	kg/m3	298.15	Partial molar volume of tertiary amines in methanol at T = 298.15 K. Solvation, shape and specific interactions

rh _{ol}	807.46	kg/m ³	298.15	Liquid-liquid equilibria, excess molar volume and deviations of the refractive indices at 298.15 K for mixtures of solvents used in the molybdenum extraction process
rh _{ol}	807.90	kg/m ³	298.15	Liquid-liquid equilibria for aqueous sulfuric acid solutions with undecane, dodecane, or 1-dodecanol, trioctylamine or tributyl phosphate and excess and deviation properties for sub-binary systems at 298.15 K
rh _{ol}	807.26	kg/m ³	298.15	Density, viscosity and excess molar volume of binary mixtures of tri-n-octylamine + diluents (n-heptane, n-octane, n-nonane, and n-decane) at various temperatures

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{\text{vap}}) = A + B/(T + C)$
Coeff. A	1.52061e+01
Coeff. B	-5.53069e+03
Coeff. C	-1.16832e+02
Temperature range (K), min.	487.56
Temperature range (K), max.	675.79

Sources

Solid-Liquid Equilibria, Excess Molar Volumes, and Molar Refractivity Deviations of Extractive Solvent Molecules and deviations of the refractive index at 298 K for the Vaporization of Equilibrium and Knudsen Dose Pressures Determined by Benzyltriethylamine, N-methanol, and a Series of Aliphatic, Saturated Amines by Correlation Gas Pressure-Graphy at T/K = 298.15: Joback Method.	https://www.doi.org/10.1021/je900586f
Density, viscosity and excess molar volume of binary mixtures of Grignard Method + diluents (n-heptane, n-octane, n-nonane, and n-decane) at various temperatures tri-n-butylphosphate or tri-octylamine contained systems; Excessive volumes of mercury sulfide sulfuric acid solutions with undecane, McGowan's book: dodecanol, trioctylamine or tributyl phosphate and excess and deviation properties for sub-binary systems at 298.15 K; Excess molar volumes and excess molar enthalpies of binary and ternary Thermo dynamics and kinetic analyses of thermal dissociation (octylamine) and n-hexane. Experimental results and PR-EoS DFT-TCA study:	https://www.doi.org/10.1016/j.fluid.2013.06.013
	https://www.doi.org/10.1021/je500358r
	https://www.doi.org/10.1016/j.jct.2012.07.012
	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure-and-thermodynamic-properties-of-chemical-substances
	https://en.wikipedia.org/wiki/Joback_method
	https://www.doi.org/10.1016/j.jct.2013.09.017
	http://pubs.acs.org/doi/abs/10.1021/ci990307l
	https://www.doi.org/10.1016/j.fluid.2010.04.016
	https://www.doi.org/10.1016/j.fluid.2013.01.002
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1116763&Units=SI
	https://www.chemeo.com/doc/models/crippen_log10ws
	https://www.doi.org/10.1016/j.jct.2005.12.006
	https://www.doi.org/10.1016/j.tca.2018.05.017
	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpolt:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc:

Critical Volume

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