

1-Pentamine, N,N-dipentyl-

Other names:	N,N-dipentyl-1-pentanamine TRI-N-PENTYLAMINE TRIPENTYLAMINE Triamylamine tri-n-Amylamine
Inchi:	InChI=1S/C15H33N/c1-4-7-10-13-16(14-11-8-5-2)15-12-9-6-3/h4-15H2,1-3H3
InchiKey:	OOHAUGDGCWURIT-UHFFFAOYSA-N
Formula:	C15H33N
SMILES:	CCCCCN(CCCCC)CCCCC
Mol. weight [g/mol]:	227.43
CAS:	621-77-2

Physical Properties

Property code	Value	Unit	Source
gf	186.20	kJ/mol	Joback Method
hf	-285.40	kJ/mol	Joback Method
hfus	37.63	kJ/mol	Joback Method
hvap	51.03	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.859		Crippen Method
mcvol	232.190	ml/mol	McGowan Method
pc	1413.31	kPa	Joback Method
rinpol	1427.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1420.00		NIST Webbook
ripol	1469.00		NIST Webbook
tb	515.65 ± 4.00	K	NIST Webbook
tb	515.70	K	NIST Webbook
tc	713.24	K	Joback Method
tf	291.28	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.67	J/mol×K	555.04	Joback Method
cpg	615.72	J/mol×K	581.41	Joback Method
cpg	634.02	J/mol×K	607.77	Joback Method
cpg	651.58	J/mol×K	634.14	Joback Method
cpg	668.42	J/mol×K	660.51	Joback Method
cpg	684.57	J/mol×K	686.87	Joback Method
cpg	700.04	J/mol×K	713.24	Joback Method
rhoI	786.41	kg/m3	298.15	Partial molar volume of tertiary amines in methanol at T = 298.15 K. Solvation, shape and specific interactions

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.57439e+01
Coeff. B	-4.79577e+03
Coeff. C	-8.46400e+01
Temperature range (K), min.	394.92
Temperature range (K), max.	544.34

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	1.54166e+01
Coeff. B	-5.89585e+03
Coeff. C	4.32624e-03
Coeff. D	-7.05007e-09
Temperature range (K), min.	298.15
Temperature range (K), max.	338.15

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermodynamic study of (heptane + amine) mixtures. III: Excess and partial molar volumes in mixtures with secondary, tertiary, and cyclic amines at 298.15 K.	https://www.doi.org/10.1016/j.jct.2011.04.017
KDB:	https://www.thermopedia.com/doc/thermdata/kdb/mol/mol1284.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C621772&Units=SI
Crippen Method:	https://www.chemed.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.thermopedia.com/doc/thermdata/kdb/hcprop/showprop.php?cmpid=1284
Partial molar volume of tertiary amines in methanol at T = 298.15 K. Solvation, shape and specific interactions:	https://www.doi.org/10.1016/j.jct.2012.07.012

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
hvac:	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
rho:	Liquid Density
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

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