

# 1-Propanamine, 2-methyl-N,N-bis(2-methylpropyl)-

Other names:	Triisobutylamine tri(2-methylpropyl)ylamine
Inchi:	InChI=1S/C12H27N/c1-10(2)7-13(8-11(3)4)9-12(5)6/h10-12H,7-9H2,1-6H3
InchiKey:	IFFFFBSAXDNJHX-UHFFFAOYSA-N
Formula:	C12H27N
SMILES:	CC(C)CN(CC(C)C)CC(C)C
Mol. weight [g/mol]:	185.35
CAS:	1116-40-1

## Physical Properties

Property code	Value	Unit	Source
chl	-8249.20	kJ/mol	NIST Webbook
gf	153.62	kJ/mol	Joback Method
hf	-239.32	kJ/mol	Joback Method
hfl	-332.00	kJ/mol	NIST Webbook
hfus	19.29	kJ/mol	Joback Method
hvap	43.19	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	3.256		Crippen Method
mcvol	189.920	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
tb	464.65 ± 0.40	K	NIST Webbook
tc	654.52	K	Joback Method
tf	251.35 ± 0.50	K	NIST Webbook
vc	0.708	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.18	J/mol×K	485.08	Joback Method
cpg	460.84	J/mol×K	513.32	Joback Method
cpg	478.72	J/mol×K	541.56	Joback Method
cpg	495.83	J/mol×K	569.80	Joback Method
cpg	512.19	J/mol×K	598.04	Joback Method

cpg	527.84	J/mol×K	626.28	Joback Method
cpg	542.79	J/mol×K	654.52	Joback Method
hvapt	52.30	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	54.30	kJ/mol	378.50	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56822e+01
Coeff. B	-4.36280e+03
Coeff. C	-7.03230e+01
Temperature range (K), min.	353.72
Temperature range (K), max.	491.01

## Sources

**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:**  
**Joback Method:**  
**McGraw Hill**  
**NIST Webbook:**

- <https://www.doi.org/10.1021/je500358r>
- [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)
- <http://link.springer.com/article/10.1007/BF02311772>
- <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1116401&Units=SI>
- <https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
- <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
- [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

# Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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