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: IIFFFBSAXDNJHX-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	512.19	J/mol×K	598.04	Joback Method
cpg	527.84	J/mol×K	626.28	Joback Method
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	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(Pvp) = 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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1116401&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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:	https://www.doi.org/10.1021/je500358r

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume