1-Dodecanamine

Other names: 1-AMINODODECANE
1-Dodecylamine
Alamine 4
Amine 12
Amine BB
Armeen 12
Armeen 12D
Dodecylamine
Farmin 20D
Kemamine P690
LAURYLAMINE
Lauramine
Laurinamine
Monododecylamine
Nissan Amine BB
n-Dodecylamine
n-Laurylamine

Inchi: InChI=1S/C12H27N/c1-2-3-4-5-6-7-8-9-10-11-12-13/h2-13H2,1H3

InchiKey: JRBPAEWTRLWTQC-UHFFFAOYSA-N

Formula: C12H27N

SMILES: CCCCCCCCCCCCN

Mol. weight [g/mol]: 185.35

CAS: 124-22-1

Physical Properties

Property code	Value	Unit	Source
basg	879.50 ± 9.20	kJ/mol	NIST Webbook
gf	116.61	kJ/mol	Joback Method
hf	-257.22	kJ/mol	Joback Method
hfus	32.03	kJ/mol	Joback Method
hvap	52.95	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.866		Crippen Method
mcvol	189.920	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinpol	1435.00		NIST Webbook
rinpol	1444.00		NIST Webbook

rinpol	1436.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1435.00		NIST Webbook
ripol	1720.00		NIST Webbook
ripol	1724.00		NIST Webbook
ripol	1725.00		NIST Webbook
ripol	1716.00		NIST Webbook
ripol	1710.00		NIST Webbook
tb	521.15 ± 5.00	K	NIST Webbook
tb	405.65 ± 5.00	K	NIST Webbook
tb	521.20	K	NIST Webbook
tb	531.15	K	KDB
tb	532.20	K	NIST Webbook
tc	718.11	K	Joback Method
tf	298.15 ± 2.00	K	NIST Webbook
tf	300.65 ± 2.00	K	NIST Webbook
tf	301.47 ± 0.50	K	NIST Webbook
tf	299.35 ± 1.50	K	NIST Webbook
tf	301.15 ± 0.50	K	NIST Webbook
tf	301.47 ± 0.50	K	NIST Webbook
tf	299.95	K	KDB
tf	301.47 ± 0.50	K	NIST Webbook
tf	301.43 ± 0.30	K	NIST Webbook
tf	301.41 ± 0.30	K	NIST Webbook
tf	301.15 ± 0.50	K	NIST Webbook
tf	299.95 ± 1.00	K	NIST Webbook
tf	301.70 ± 1.50	K	NIST Webbook
tf	302.00 ± 3.00	K	NIST Webbook
tf	300.65 ± 0.50	K	NIST Webbook
vc	0.737	m3/kmol	Joback Method
volm	2.32e-04	m3/mol	Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.85	J/mol×K	546.49	Joback Method

cpg	496.61	J/mol×K	575.09	Joback Method
cpg	512.68	J/mol×K	603.70	Joback Method
cpg	528.07	J/mol×K	632.30	Joback Method
cpg	542.80	J/mol×K	660.90	Joback Method
cpg	556.89	J/mol×K	689.50	Joback Method
cpg	570.37	J/mol×K	718.11	Joback Method
hvapt	63.40	kJ/mol	438.50	NIST Webbook
psub	1.60e-03	kPa	298.15	The Vaporization Enthalpies and Vapor Pressures of Some Primary Amines of Pharmaceutical Importance by Correlation Gas Chromatography

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	399.70	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.67994e+01
Coeff. B	-5.26293e+03
Coeff. C	-8.91430e+01
Temperature range (K), min.	407.88
Temperature range (K), max.	547.27

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.81347e+02
Coeff. B	-1.55663e+04
Coeff. C	-2.40572e+01
Coeff. D	1.24413e-05

Temperature range (K), min.	301.47
Temperature range (K), max.	696.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1281
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C124221&Units=SI
The Vaporization Enthalpies and Vapor Pressures of Some Primary Amines of Pharmaceutical Importance by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je400498a
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1281.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K:	https://www.doi.org/10.1016/j.jct.2010.12.025
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

basg:	Gas basicity
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
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
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

volm: Molar Volume

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