Caprolactam

Other names:

.epsilon.-caprolactam
.omega.-caprolactam
1,6-Hexolactam
1-Aza-2-cycloheptanone
2-Azacycloheptanone
2-Azepanone
2-Ketohexamethyleneimine
2-Ketohexamethylenimine
2-Oxohexamethyleneimine
2-Oxohexamethylenimine
2-Perhydroazepinone
2H-Azepin-2-one, hexahydro-
2H-Azepin-7-one, hexahydro-
6-Aminocaproic acid lactam
6-Aminohexanoic acid cyclic lactam
6-Aminohexanoic acid lactam
6-Caprolactam
6-Hexanelactam
6-aminohexanoic acid, .epsilon.-lactam
A1030
ATM 2(NYLON)
Akulon
Alkamid
Amilan cm 1001
Amilan cm 1001C
Amilan cm 1001G
Amilan cm 1011
Aminocaproic lactam
Azepan-2-one
Bonamid
CM 1001
CM 1011
CM 1031
CM 1041
Capran 77C
Capran 80
Caprolattame
Caprolon B
Caprolon V
Capron

Capron 8250
Capron 8252
Capron 8253
Capron 8256
Capron 8257
Capron B
Capron GR 8256
Capron GR 8258
Capron PK4
Chemlon
Danamid
Dull 704
Durethan bk
Durethan bk 30S
Durethan bkv 30H
Durethan bkv 55H
EPSILON-CAPROLACTAM
Epsylon kaprolaktam
Ertalon 6sa
Extrom 6N
Grilon
Hexahydro-2-azepinone
Hexahydro-2H-azepin-2-one
Hexamethylenimine, 2-oxo-
Hexano-6-lactam
Hexanoic acid, 6-amino-, cyclic lactam
Hexanoic acid, 6-amino-, lactam
Hexanolactam
Hexanonisoxim
Itamid
Itamid 250
Itamide 25
Itamide 250
Itamide 250G
Itamide 35
Itamide 350
Itamide S
Kaprolit
Kaprolit B
Kaprolon
Kaprolon B
Kapromine
Kapron

Kapron A
Kapron B
Maranyl F 114
Maranyl F 124
Maranyl F 500
Metamid
Miramid H 2
Miramid wm 55
NCI-C50646
Nylon A1035sf
Nylon X 1051
Nylon cm 1031
Orgamid RMNOCD
Orgamide
PA 6
PK 4
PKA
Plaskin 8200
Plaskon 201
Plaskon 8201
Plaskon 8201hs
Plaskon 8202C
Plaskon 8205
Plaskon 8207
Plaskon 8252
Plaskon xp 607
Polyamide pk 4
Relon P
Renyl MV
Sipas 60
Spencer 401
Spencer 601
Steelon
Stilon
Stylon
Tarlon X-A
Tarlon XB
Tarnamid T
Tarnamid T 2
Tarnamid T 27
Torayca N 6
UBE 1022B
Ultramid B 3

	Ultramid B 4
	Ultramid B 5
	Ultramid BMK
	Vidlon
	Widlon
	Zytel 211
	caproic acid, 6-amino, .epsilon.-lactam
	hexanoic acid, 6-amino, .epsilon.-lactam
	«epsilon»-Caprolactam
	«omega»-Caprolactam
	Â«epsilonÂ»-Caprolactam
	Â«omegaÂ»-Caprolactam
Inchi:	InChI=1S/C6H11NO/c8-6-4-2-1-3-5-7-6/h1-5H2,(H,7,8)
InchiKey:	JBKVHLHDHHXQEQ-UHFFFAOYSA-N
Formula:	C6H11NO
SMILES:	O=C1CCCCCN1
Mol. weight [g/mol]:	113.16
CAS:	105-60-2

Physical Properties

Property code	Value	Unit	Source
chs	-3603.80 ± 1.50	kJ/mol	NIST Webbook
chs	-3603.70 ± 0.84	kJ/mol	NIST Webbook
chs	-3588.00 ± 6.30	kJ/mol	NIST Webbook
gf	-15.18	kJ/mol	Joback Method
hf	-239.60	kJ/mol	NIST Webbook
hfs	-329.40 ± 1.70	kJ/mol	NIST Webbook
hfus	16.16	kJ/mol	Solid-Liquid Equilibrium and Activity Coefficients for Caprolactam + 1-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide and Cyclohexanone Oxime + 1-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide
hsub	87.30 ± 0.20	kJ/mol	NIST Webbook
hsub	89.76 ± 0.81	kJ/mol	NIST Webbook
hvap	40.86	kJ/mol	Joback Method
ie	9.07 ± 0.02	eV	NIST Webbook
ie	9.19	eV	NIST Webbook
log10ws	-1.19		Crippen Method

logp	0.677		Crippen Method
mcvol	96.090	ml/mol	McGowan Method
pc	4621.41	kPa	Joback Method
rinpol	215.49		NIST Webbook
rinpol	1252.90		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	217.00		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1252.90		NIST Webbook
rinpol	215.49		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1255.00		NIST Webbook
ss	173.21	J/mol×K	NIST Webbook
ss	168.60	J/mol×K	NIST Webbook
ss	168.60	J/mol×K	NIST Webbook
ss	168.40	J/mol×K	NIST Webbook
tb	481.54	K	Joback Method
tc	801.00	K	Critical temperatures and pressures of caprolactam, dimethyl sulfoxide, 1,4-dimethylpiperazine, and 2,6-dimethylpiperazine
tf	342.35 ± 0.03	K	NIST Webbook
tf	342.30 ± 0.50	K	NIST Webbook
tf	342.25	K	NIST Webbook
tf	342.21	K	Thermodynamics of Mixtures Containing a Strongly Polar Compound. 9. Liquid-Liquid Equilibria for epsilon-Caprolactam + Selected Alkanes
tf	342.20 ± 0.50	K	NIST Webbook
tt	342.31 ± 0.01	K	NIST Webbook
tt	342.30 ± 0.01	K	NIST Webbook
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.47	J/mol×K	603.46	Joback Method
cpg	231.29	J/mol×K	562.82	Joback Method
cpg	216.38	J/mol×K	522.18	Joback Method

cpg	283.37	J/mol×K	725.38	Joback Method
cpg	271.55	J/mol×K	684.74	Joback Method
cpg	258.90	J/mol×K	644.10	Joback Method
cpg	200.77	J/mol×K	481.54	Joback Method
cps	156.78	J/mol×K	298.15	NIST Webbook
cps	156.77	J/mol×K	298.15	NIST Webbook
cps	158.10	J/mol×K	300.00	NIST Webbook
cps	156.30	J/mol×K	300.00	NIST Webbook
hfust	16.10	kJ/mol	342.31	NIST Webbook
hfust	16.10	kJ/mol	342.31	NIST Webbook
hfust	16.16	kJ/mol	342.20	NIST Webbook
hfust	16.20	kJ/mol	342.30	NIST Webbook
hfust	16.10	kJ/mol	343.30	NIST Webbook
hfust	16.13	kJ/mol	342.36	NIST Webbook
hfust	16.10	kJ/mol	342.31	NIST Webbook
hfust	16.10	kJ/mol	343.30	NIST Webbook
hsubt	86.30 ± 0.20	kJ/mol	338.00	NIST Webbook
hsubt	86.30	kJ/mol	315.50	NIST Webbook
hsubt	86.90	kJ/mol	320.50	NIST Webbook
hsubt	89.30 ± 0.80	kJ/mol	335.00	NIST Webbook
hsubt	77.50	kJ/mol	283.00	NIST Webbook
hsubt	83.30 ± 0.80	kJ/mol	304.00	NIST Webbook
hvapt	52.40 ± 0.50	kJ/mol	459.00	NIST Webbook
hvapt	69.20 ± 0.30	kJ/mol	459.00	NIST Webbook
hvapt	65.70 ± 0.30	kJ/mol	459.00	NIST Webbook
hvapt	87.60	kJ/mol	350.03	Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam
hvapt	59.00 ± 0.20	kJ/mol	459.00	NIST Webbook
hvapt	62.30	kJ/mol	458.00	NIST Webbook
hvapt	87.26	kJ/mol	298.15	NIST Webbook
hvapt	62.30 ± 0.20	kJ/mol	459.00	NIST Webbook
hvapt	55.70 ± 0.30	kJ/mol	459.00	NIST Webbook
psub	4.74e-04	kPa	303.32	Thermodynamics of the Sublimation and of the Vaporization of e-Caprolactam
psub	6.36e-03	kPa	327.93	Thermodynamics of the Sublimation and of the Vaporization of e-Caprolactam

psub	6.10e-03	kPa	328.00	Thermodynamics of the Sublimation and of the Vaporization of e-Caprolactam
psub	0.01	kPa	332.89	Thermodynamics of the Sublimation and of the Vaporization of e-Caprolactam
psub	0.01	kPa	332.93	Thermodynamics of the Sublimation and of the Vaporization of e-Caprolactam
psub	0.02	kPa	337.82	Thermodynamics of the Sublimation and of the Vaporization of e-Caprolactam
psub	3.93e-03	kPa	322.98	Thermodynamics of the Sublimation and of the Vaporization of e-Caprolactam
psub	2.35e-03	kPa	318.09	Thermodynamics of the Sublimation and of the Vaporization of e-Caprolactam
psub	1.53e-04	kPa	293.43	Thermodynamics of the Sublimation and of the Vaporization of e-Caprolactam
psub	1.43e-03	kPa	313.22	Thermodynamics of the Sublimation and of the Vaporization of e-Caprolactam
psub	8.58e-04	kPa	308.38	Thermodynamics of the Sublimation and of the Vaporization of e-Caprolactam
psub	8.13e-04	kPa	308.31	Thermodynamics of the Sublimation and of the Vaporization of e-Caprolactam

psub	3.79e-03	kPa	323.06	Thermodynamics of the Sublimation and of the Vaporization of e-Caprolactam
psub	2.75e-04	kPa	298.39	Thermodynamics of the Sublimation and of the Vaporization of e-Caprolactam
pvap	0.05	kPa	353.00	Solid-Liquid Equilibrium and Activity Coefficients for Binary Mixtures of Caprolactam and Cyclohexanone Oxime with Room-Temperature Ionic Liquids
pvap	0.03	kPa	343.00	Solid-Liquid Equilibrium and Activity Coefficients for Binary Mixtures of Caprolactam and Cyclohexanone Oxime with Room-Temperature Ionic Liquids
pvap	0.04	kPa	347.90	Solid-Liquid Equilibrium and Activity Coefficients for Binary Mixtures of Caprolactam and Cyclohexanone Oxime with Room-Temperature Ionic Liquids
pvap	0.04	kPa	348.00	Solid-Liquid Equilibrium and Activity Coefficients for Binary Mixtures of Caprolactam and Cyclohexanone Oxime with Room-Temperature Ionic Liquids

pvap	0.05	kPa	352.90	Solid-Liquid Equilibrium and Activity Coefficients for Binary Mixtures of Caprolactam and Cyclohexanone Oxime with Room-Temperature Ionic Liquids
sfust	47.00	J/mol×K	342.31	NIST Webbook
sfust	47.00	J/mol×K	342.31	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	410.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.13763e+02
Coeff. B	-1.26926e+04
Coeff. C	-1.38483e+01
Coeff. D	4.82981e-06
Temperature range (K), min.	342.36
Temperature range (K), max.	806.00

Sources

Solid-Liquid Equilibrium and Activity Coefficients for Binary Mixtures of Caprolactam and Cyclohexanone Oxime with Room-Temperature Ionic Liquids:	https://www.doi.org/10.1021/je1005054
Critical temperatures and pressures of caprolactam + dimethyl sulfoxide, + 1,3-dimethylpiperazine, and 2,6-dimethylpiperazine:	https://www.doi.org/10.1016/j.fluid.2018.05.029
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1471
Determination and modeling for solid-liquid phase equilibrium of ternary ε-caprolactam + cyclohexanone oxime + methyl tert-butyl ether system:	https://www.doi.org/10.1016/j.fluid.2016.03.002
Thermodynamics of Mixtures Containing Strongly Polar Compound. 9. Liquid-Liquid Equilibria for epsilon-Caprolactam + Selected Alkanes:	https://www.doi.org/10.1021/je900785z

Thermodynamic properties of epsilon-caprolactam and epsilon-caprothiolactam:	https://www.doi.org/10.1016/j.jct.2019.01.014
Experimental Study of Thermodynamic Properties of Mixtures Containing Ionic Liquid 1-Ethyl-3-methylimidazolium Ethyl Sulfate Using Gas-Liquid Chromatography and Transpiration Method:	https://www.doi.org/10.1021/je0602723
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Density, Viscosity, and Surface Tension of Liquid Phase Beckmann Rearrangement Mixtures:	https://www.doi.org/10.1021/je500836b
Thermodynamics of the Sublimation and of the Vaporization of ε-Caprolactam:	https://www.doi.org/10.1021/je050277k
Solubility of caprolactam in different organic solvents:	https://www.doi.org/10.1016/j.fluid.2011.12.004
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solid-Liquid Equilibrium and Activity Coefficients for Caprolactam + 1-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide and Cyclohexanone Oxime + 1-Hexyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1021/je7000683
Solubility of SO2 in Caprolactam + Tetrabutylammonium Bromide Ionic Liquids:	https://www.doi.org/10.1021/je900565e
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1471.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Electrical Conductivity of Caprolactam + Tetrabutylammonium Bromide Ionic Liquids in Aqueous and Alcohol Binary Systems:	https://www.doi.org/10.1021/je100361s
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105602&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume