Acetamide

Other names:	Acetic acid amide
	Amid kyseliny octove
	CH3CONH2
	Ethanamide
	Methanecarboxamide
	NCI-C02108
	acetimidic acid
Inchi:	InChI=1S/C2H5NO/c1-2(3)4/h1H3,(H2,3,4)
InchiKey:	DLFVBJFMPXGRIB-UHFFFAOYSA-N
Formula:	C2H5NO
SMILES:	CC(N)=O
Mol. weight [g/mol]:	59.07
CAS:	60-35-5

Physical Properties

Property code	Value	Unit	Source
affp	863.60	kJ/mol	NIST Webbook
basg	832.60	kJ/mol	NIST Webbook
chs	-1191.50	kJ/mol	NIST Webbook
chs	-1184.60 ± 0.69	kJ/mol	NIST Webbook
chs	-1186.03 ± 0.82	kJ/mol	NIST Webbook
gf	-96.51	kJ/mol	Joback Method
hf	-238.33 ± 0.78	kJ/mol	NIST Webbook
hfs	-315.60 ± 0.82	kJ/mol	NIST Webbook
hfs	-310.10	kJ/mol	NIST Webbook
hfs	-316.99 ± 0.70	kJ/mol	NIST Webbook
hfus	7.73	kJ/mol	Joback Method
hsub	80.00 ± 1.00	kJ/mol	NIST Webbook
hsub	80.30 ± 1.30	kJ/mol	NIST Webbook
hsub	77.20	kJ/mol	NIST Webbook
hsub	80.00 ± 1.00	kJ/mol	NIST Webbook
hsub	78.66 ± 0.33	kJ/mol	NIST Webbook
hvap	37.43	kJ/mol	Joback Method
ie	9.65 ± 0.03	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	9.62	eV	NIST Webbook

ie	9.62	eV	NIST Webbook
ie	9.70	eV	NIST Webbook
ie	10.15 ± 0.05	eV	NIST Webbook
ie	9.69 ± 0.07	eV	NIST Webbook
ie	9.77 ± 0.02	eV	NIST Webbook
log10ws	1.58		Aqueous Solubility Prediction Method
log10ws	1.58		Estimated Solubility Method
logp	-0.508		Crippen Method
mcvol	50.590	ml/mol	McGowan Method
pc	6009.25	kPa	Joback Method
rinpol	764.00		NIST Webbook
rinpol	719.80		NIST Webbook
ripol	1775.00		NIST Webbook
ripol	1738.00		NIST Webbook
ripol	1788.00		NIST Webbook
ripol	1763.00		NIST Webbook
ripol	1725.00		NIST Webbook
ripol	1763.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1788.00		NIST Webbook
ss	115.00	J/mol×K	NIST Webbook
ss	115.00	J/mol×K	NIST Webbook
tb	494.30 ± 0.25	K	NIST Webbook
tb	494.40 ± 1.00	K	NIST Webbook
tb	494.30 ± 0.50	K	NIST Webbook
tb	494.30	K	KDB
tb	494.40	K	NIST Webbook
tb	495.00	K	NIST Webbook
tb	494.30 ± 0.80	K	NIST Webbook
tc	569.97	K	Joback Method
tf	353.40	K	Aqueous Solubility Prediction Method
tf	354.90 ± 0.20	K	NIST Webbook
tf	342.00 ± 2.00	K	NIST Webbook
tf	352.85 ± 0.50	K	NIST Webbook
tf	355.50 ± 0.50	K	NIST Webbook
tf	353.50 ± 0.20	K	NIST Webbook
tf	352.00 ± 1.00	K	NIST Webbook
tt	353.33 ± 0.02	K	NIST Webbook
vc	0.182	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	85.13	J/mol×K	371.56	Joback Method
cpg	107.81	J/mol×K	536.91	Joback Method
cpg	103.67	J/mol×K	503.84	Joback Method
cpg	99.33	J/mol×K	470.77	Joback Method
cpg	94.80	J/mol×K	437.70	Joback Method
cpg	90.07	J/mol×K	404.63	Joback Method
cpg	111.77	J/mol×K	569.97	Joback Method
cps	90.30	J/mol×K	298.15	NIST Webbook
cps	90.00	J/mol×K	300.00	NIST Webbook
cps	91.27	J/mol×K	298.15	NIST Webbook
cps	91.27	J/mol×K	298.15	NIST Webbook
cps	86.65	J/mol×K	298.00	NIST Webbook
cps	66.50	J/mol×K	293.00	NIST Webbook
hfust	15.60	kJ/mol	353.00	NIST Webbook
hfust	15.59	kJ/mol	353.33	NIST Webbook
hfust	15.61	kJ/mol	353.50	NIST Webbook
hfust	12.70 ± 0.18	kJ/mol	342.15	NIST Webbook
hfust	15.50	kJ/mol	354.05	NIST Webbook
hsubt	77.80	kJ/mol	283.00	NIST Webbook
hsubt	77.40 ± 0.40	kJ/mol	323.50	NIST Webbook
hvapt	60.90	kJ/mol	416.50	NIST Webbook
hvapt	63.80	kJ/mol	436.50	NIST Webbook
sfust	44.10	J/mol×K	353.33	NIST Webbook
sfust	44.15	J/mol×K	353.50	NIST Webbook
sfust	37.10 ± 0.50	J/mol×K	342.15	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.00	K	0.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50381e+01
Coeff. B	-4.16112e+03
Coeff. C	-9.50520e+01
Temperature range (K), min.	354.15
Temperature range (K), max.	522.86

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.60285e+01
Coeff. B	-9.50648e+03
Coeff. C	-6.90968e+00
Coeff. D	2.70255e-06
Temperature range (K), min.	354.15
Temperature range (K), max.	545.15

Sources

Densities and viscosities of, and NH3 solubilities in deep eutectic solvents composed of ethylamine hydrochloride and acetamide:	https://www.doi.org/10.1016/j.jct.2019.105883
KDB, Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1375
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Enthalpies of Dilution of Acetamide and N,N-Dimethylformamide in Aqueous Sodium Chloride Solutions at 298.15 K:	https://www.doi.org/10.1021/je8000393
Influence of aliphatic amides on the temperature of maximum density of water:	https://www.doi.org/10.1016/j.jct.2016.10.024
Properties for binary mixtures of (acetamide + KSCN) eutectic ionic liquid with ethanol at several temperatures:	https://www.doi.org/10.1016/j.jct.2015.08.036
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60355&Units=SI
Specific Conductivities and Viscosities of 0.1LiNO3 + 0.9[xCH3CONH2 + (1 x)CO(NH2)2] as Functions of Mole Fraction, x, and Temperature:	https://www.doi.org/10.1021/je300707j
Solubility of Acetamide, Propionamide, and Butyramide in Water at Temperatures between (278.15 and 333.15) K:	https://www.doi.org/10.1021/je9007475
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Enthalpy of dilution of aliphatic amides in aqueous solutions at temperatures between 293.15K and 308.15K:	https://www.doi.org/10.1016/j.tca.2009.01.021
Measurement and correlation of the solubility of 3,4-bis(3-nitrofurazan-4-yl)furoxan (DNTF) in different solvents:	https://www.doi.org/10.1016/j.jct.2015.06.003
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Measurement of Activity Coefficients of Solutes at Infinite Dilution in (Dimethyl Sulfoxide + Acetamide, or Formamide, or Urea) Using Gas Liquid Chromatography at the Temperature 298.15 K:	https://www.doi.org/10.1021/je030122h
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubility of Ethanamide and 2-Propenamide in Supercritical Carbon Dioxide. Measurements and Correlation:	https://www.doi.org/10.1021/je900109b
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1375

Legend

affp:	Proton affinity
basg:	Gas basicity
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	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