Propanamide

Other names:	Amid kyseliny propionove
	Propionic amide
	propionamide
	propionic acid amide
Inchi:	InChI=1S/C3H7NO/c1-2-3(4)5/h2H2,1H3,(H2,4,5)
InchiKey:	QLNJFJADRCOGBJ-UHFFFAOYSA-N
Formula:	C3H7NO
SMILES:	CCC(N)=O
Mol. weight [g/mol]:	73.09
CAS:	79-05-0

Physical Properties

Property code	Value	Unit	Source
affp	876.20	kJ/mol	NIST Webbook
basg	845.30	kJ/mol	NIST Webbook
basg	847.30 ± 5.00	kJ/mol	NIST Webbook
basg	844.40 ± 4.90	kJ/mol	NIST Webbook
basg	845.00 ± 10.00	kJ/mol	NIST Webbook
basg	845.00 ± 10.00	kJ/mol	NIST Webbook
basg	843.30 ± 3.00	kJ/mol	NIST Webbook
basg	843.10 ± 4.10	kJ/mol	NIST Webbook
gf	-88.09	kJ/mol	Joback Method
hf	-258.94 ± 0.66	kJ/mol	NIST Webbook
hfus	12.90	kJ/mol	Heat Capacities and Enthalpies of Solid-Solid Transitions and Fusion of a Series of Eleven Primary Alkylamides by Differential Scanning Calorimetry
hfus	68.70	kJ/mol	Validation of the Vaporization Enthalpies of Some Simple Aliphatic Amides and Their Use in the Evaluation of the Vaporization Enthalpy of Valpromide and Valnoctamide
hsub	75.00 ± 4.00	kJ/mol	NIST Webbook
hsub	79.25 ± 0.33	kJ/mol	NIST Webbook
hvap	39.66	kJ/mol	Joback Method
log10ws	-0.29		Crippen Method

logp	-0.118		Crippen Method
mcvol	64.680	ml/mol	McGowan Method
pc	5205.63	kPa	Joback Method
rinpol	984.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1801.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1801.00		NIST Webbook
ripol	1821.00		NIST Webbook
ripol	1792.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1792.00		NIST Webbook
tb	486.20	K	NIST Webbook
tb	495.40 ± 0.80	K	NIST Webbook
tb	495.35 ± 1.50	K	NIST Webbook
tb	495.30 ± 0.50	K	NIST Webbook
tb	495.30 ± 0.50	K	NIST Webbook
tc	591.47	K	Joback Method
tf	352.80 ± 0.60	K	NIST Webbook
vc	0.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.34	J/mol×K	460.12	Joback Method
cpg	124.01	J/mol×K	427.28	Joback Method
cpg	152.96	J/mol×K	591.47	Joback Method
cpg	147.69	J/mol×K	558.63	Joback Method
cpg	142.17	J/mol×K	525.79	Joback Method
cpg	136.39	J/mol×K	492.95	Joback Method
cpg	117.40	J/mol×K	394.44	Joback Method
hfust	12.90	kJ/mol	352.60	NIST Webbook
hfust	12.90	kJ/mol	352.60	NIST Webbook
hsubt	79.10 ± 0.40	kJ/mol	332.00	NIST Webbook
hvapt	60.30	kJ/mol	412.00	NIST Webbook
hvapt	63.90	kJ/mol	425.50	NIST Webbook

pvap	31.04	kPa	455.55	Vapor-Liquid-Liquid Equilibria, Azeotropic, and Excess Enthalpy Data for the Binary System n-Undecane + Propionamide, and Pure Component Vapor Pressure and Density Data for Propionamide
pvap	60.86	kPa	475.85	Vapor-Liquid-Liquid Equilibria, Azeotropic, and Excess Enthalpy Data for the Binary System n-Undecane + Propionamide, and Pure Component Vapor Pressure and Density Data for Propionamide
pvap	11.22	kPa	427.65	Vapor-Liquid-Liquid Equilibria, Azeotropic, and Excess Enthalpy Data for the Binary System n-Undecane + Propionamide, and Pure Component Vapor Pressure and Density Data for Propionamide
pvap	6.40	kPa	414.05	Vapor-Liquid-Liquid Equilibria, Azeotropic, and Excess Enthalpy Data for the Binary System n-Undecane + Propionamide, and Pure Component Vapor Pressure and Density Data for Propionamide

pvap	4.02	kPa	403.65	Vapor-Liquid-Liquid Equilibria, Azeotropic, and Excess Enthalpy Data for the Binary System n-Undecane + Propionamide, and Pure Component Vapor Pressure and Density Data for Propionamide
pvap	2.52	kPa	394.15	Vapor-Liquid-Liquid Equilibria, Azeotropic, and Excess Enthalpy Data for the Binary System n-Undecane + Propionamide, and Pure Component Vapor Pressure and Density Data for Propionamide
pvap	1.53	kPa	384.15	Vapor-Liquid-Liquid Equilibria, Azeotropic, and Excess Enthalpy Data for the Binary System n-Undecane + Propionamide, and Pure Component Vapor Pressure and Density Data for Propionamide
pvap	0.97	kPa	375.45	Vapor-Liquid-Liquid Equilibria, Azeotropic, and Excess Enthalpy Data for the Binary System n-Undecane + Propionamide, and Pure Component Vapor Pressure and Density Data for Propionamide

pvap	50.69	kPa	469.05	Vapor-Liquid-Liquid Equilibria, Azeotropic, and Excess Enthalpy Data for the Binary System n-Undecane + Propionamide, and Pure Component Vapor Pressure and Density Data for Propionamide
pvap	21.16	kPa	443.85	Vapor-Liquid-Liquid Equilibria, Azeotropic, and Excess Enthalpy Data for the Binary System n-Undecane + Propionamide, and Pure Component Vapor Pressure and Density Data for Propionamide
pvap	40.87	kPa	462.95	Vapor-Liquid-Liquid Equilibria, Azeotropic, and Excess Enthalpy Data for the Binary System n-Undecane + Propionamide, and Pure Component Vapor Pressure and Density Data for Propionamide

Sources

Validation of the Vaporization Enthalpies of Some Simple Aliphatic Amides and Their Use in the Evaluation of the Vaporization Enthalpy of Valpromide and Valnoctamide:	https://www.doi.org/10.1021/je3012452
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Vapor-Liquid-Liquid Equilibria, Azeotropic, and Excess Enthalpy Data for the Binary System n-Undecane + Propionamide, and Pure Component Vapor Pressure and Density Data for Propionamide:	https://www.doi.org/10.1021/je034255e
Experimental Measurements and Correlation of the Solubility of Three Propionamide and Butanamide:	https://www.doi.org/10.1021/je400357t
influence of aliphatic amides on the temperature of maximum density of water:	https://www.doi.org/10.1016/j.jct.2016.10.024
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79050&Units=SI
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
Heat Capacities and Enthalpies of Solid-Solid Transitions and Fusion of a Series of Eleven Primary Alkylamides by Differential Scanning Calorimetry:	https://www.doi.org/10.1021/je700662a

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Solubility of Acetamide, Propionamide, and Butyramide in Water at Temperatures between (278.15 and 333.15) K: https://www.doi.org/10.1021/je9007475

Legend

affp:	Proton affinity
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
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume