2-Propenamide

Other names:	2-Propeneamide
	Acrylamide
	Acrylic amide
	Akrylamid
	Amid kyseliny akrylove
	CH2CHCONH2
	Ethylenecarboxamide
	NSC 7785
	Propenamide
	Propenoic acid, amide
	Rcra waste number U007
	UN 2074
	Vinyl amide
Inchi:	InChI=1S/C3H5NO/c1-2-3(4)5/h2H,1H2,(H2,4,5)
InchiKey:	HRPVXLWXLXDGHG-UHFFFAOYSA-N
Formula:	C3H5NO
SMILES:	C=CC(N)=O
Mol. weight [g/mol]:	71.08
CAS:	79-06-1

Physical Properties

Property code	Value	Unit	Source
affp	870.70	kJ/mol	NIST Webbook
basg	839.80	kJ/mol	NIST Webbook
chs	-1683.02 ± 0.26	kJ/mol	NIST Webbook
gf	-0.25	kJ/mol	Joback Method
hf	-130.20 ± 1.70	kJ/mol	NIST Webbook
hfl	-224.00	kJ/mol	NIST Webbook
hfs	-212.08 ± 0.30	kJ/mol	NIST Webbook
hfus	9.04	kJ/mol	Joback Method
hvap	38.99	kJ/mol	Joback Method
ie	9.50	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	9.99	eV	NIST Webbook
log10ws	0.97		Aqueous Solubility Prediction Method

logp	-0.342		Crippen Method
mcvol	60.380	ml/mol	McGowan Method
pc	5536.07	kPa	Joback Method
ripol	1943.00		NIST Webbook
tb	391.12	K	Joback Method
tc	592.61	K	Joback Method
tf	357.32	K	Aqueous Solubility Prediction Method
vc	0.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	133.86	J/mol×K	592.61	Joback Method
cpg	129.46	J/mol×K	559.03	Joback Method
cpg	124.81	J/mol×K	525.45	Joback Method
cpg	119.89	J/mol×K	491.87	Joback Method
cpg	114.69	J/mol×K	458.28	Joback Method
cpg	109.21	J/mol×K	424.70	Joback Method
cpg	103.43	J/mol×K	391.12	Joback Method
cps	110.58	J/mol×K	298.15	NIST Webbook
hfust	15.33	kJ/mol	358.00	NIST Webbook
hfust	15.33	kJ/mol	358.00	NIST Webbook
hfust	15.33	kJ/mol	358.00	NIST Webbook
hsubt	81.81	kJ/mol	330.00	NIST Webbook
hsubt	81.80	kJ/mol	330.50	NIST Webbook
hvapt	61.50	kJ/mol	385.00	NIST Webbook
hvapt	76.50	kJ/mol	393.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.20	K	3.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	-3.50162e+03
Coeff. B	1.42129e+05
Coeff. C	5.38494e+02
Coeff. D	-4.94163e-04
Temperature range (K), min.	357.65
Temperature range (K), max.	476.50

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1381
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79061&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1381
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of Ethanamide and 2-Propenamide in Supercritical Carbon Dioxide: Measurements and Correlation:	https://www.doi.org/10.1021/je900109b
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hfl:	Liquid phase 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
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
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