Pentanamide

Other names:	n-valeramide
	pentanimidic acid
	valeramide
Inchi:	InChI=1S/C5H11NO/c1-2-3-4-5(6)7/h2-4H2,1H3,(H2,6,7)
InchiKey:	IPWFJLQDVFKJDU-UHFFFAOYSA-N
Formula:	C5H11NO
SMILES:	CCCCC(N)=O
Mol. weight [g/mol]:	101.15
CAS:	626-97-1

Physical Properties

Property code	Value	Unit	Source
chs	-3160.10 ± 1.00	kJ/mol	NIST Webbook
gf	-71.25	kJ/mol	Joback Method
hf	-225.32	kJ/mol	Joback Method
hfus	75.90	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
hfus	17.90	kJ/mol	Heat Capacities and Enthalpies of Solid-Solid Transitions and Fusion of a Series of Eleven Primary Alkylamides by Differential Scanning Calorimetry
hsub	89.30 ± 0.40	kJ/mol	NIST Webbook
hvap	44.11	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	0.662		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
rinpol	918.00		NIST Webbook
rinpol	918.00		NIST Webbook
ripol	2006.00		NIST Webbook
tb	440.20	K	Joback Method
tc	633.63	K	Joback Method
tf	379.00 ± 0.60	K	NIST Webbook

vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.59	J/mol×K	536.92	Joback Method
cpg	224.87	J/mol×K	569.15	Joback Method
cpg	232.77	J/mol×K	601.39	Joback Method
cpg	189.30	J/mol×K	440.20	Joback Method
cpg	198.81	J/mol×K	472.44	Joback Method
cpg	207.90	J/mol×K	504.68	Joback Method
cpg	240.29	J/mol×K	633.63	Joback Method
hfust	17.90	kJ/mol	377.20	NIST Webbook
hsubt	89.10	kJ/mol	363.00	NIST Webbook
hsubt	89.30 ± 0.40	kJ/mol	353.50	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
Heat Capacities and Enthalpies of Solid-Solid Transitions and Fusion of a Goback Method Primary Alkylamides by Differential Scanning Calorimetry:	https://www.doi.org/10.1021/je700662a
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C626971&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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