Butanamide

Other names:	butanoic acid amide
	butyramide
	n-Butylamide
	n-Butyramide
	n-C3H7C(O)NH2
Inchi:	InChI=1S/C4H9NO/c1-2-3-4(5)6/h2-3H2,1H3,(H2,5,6)
InchiKey:	DNSISZSEWVHGLH-UHFFFAOYSA-N
Formula:	C4H9NO
SMILES:	CCCC(N)=O
Mol. weight [g/mol]:	87.12
CAS:	541-35-5

Physical Properties

Property code	Value	Unit	Source
basg	847.00 ± 6.00	kJ/mol	NIST Webbook
basg	849.00 ± 5.00	kJ/mol	NIST Webbook
chs	-2496.30 ± 0.40	kJ/mol	NIST Webbook
chs	-2494.70 ± 0.70	kJ/mol	NIST Webbook
gf	-79.67	kJ/mol	Joback Method
hf	-279.10 ± 1.80	kJ/mol	NIST Webbook
hf	-279.17 ± 0.88	kJ/mol	NIST Webbook
hfs	-365.53 ± 0.76	kJ/mol	NIST Webbook
hfs	-364.00 ± 0.40	kJ/mol	NIST Webbook
hfus	72.30	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	19.20	kJ/mol	Heat Capacities and Enthalpies of Solid-Solid Transitions and Fusion of a Series of Eleven Primary Alkylamides by Differential Scanning Calorimetry
hsub	85.40 ± 1.70	kJ/mol	NIST Webbook
hsub	85.00 ± 2.00	kJ/mol	NIST Webbook
hsub	82.00 ± 4.00	kJ/mol	NIST Webbook
hsub	82.00 ± 4.00	kJ/mol	NIST Webbook

hsub	86.36 ± 0.42	kJ/mol	NIST Webbook
hvap	41.89	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.272		Crippen Method
mcvol	78.770	ml/mol	McGowan Method
pc	4553.06	kPa	Joback Method
ripol	1901.00		NIST Webbook
ripol	1901.00		NIST Webbook
tb	489.20	K	NIST Webbook
tc	612.66	K	Joback Method
tf	388.40	K	Establishing benchmarks for the Second Industrial Fluids Simulation Challenge
tf	388.80 ± 0.50	K	NIST Webbook
vc	0.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.51	J/mol×K	514.99	Joback Method
cpg	182.61	J/mol×K	547.55	Joback Method
cpg	195.83	J/mol×K	612.66	Joback Method
cpg	189.38	J/mol×K	580.10	Joback Method
cpg	152.16	J/mol×K	417.32	Joback Method
cpg	160.30	J/mol×K	449.88	Joback Method
cpg	168.08	J/mol×K	482.43	Joback Method
hfust	19.20	kJ/mol	387.30	NIST Webbook
hfust	19.20	kJ/mol	387.30	NIST Webbook
hsubt	87.00 ± 0.80	kJ/mol	319.50	NIST Webbook
hsubt	86.40 ± 0.40	kJ/mol	359.00	NIST Webbook
hsubt	87.00	kJ/mol	363.00	NIST Webbook
hvapt	64.00	kJ/mol	450.50	NIST Webbook

Sources

Establishing benchmarks for the Second Industrial Fluids Simulation Challenge:	https://www.doi.org/10.1016/j.fluid.2005.04.020
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C541355&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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
Solubility of Acetamide, Propionamide, and Butyramide in Water at Temperatures between (278.15 and 338.15) K:	https://www.doi.org/10.1021/je9007475
Experimental Measurements and Correlation of the Solubility of Three Primary Amides in Supercritical CO2:	https://www.doi.org/10.1021/je400357t
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Acetanilide, Propanamide, and Butanamide:	https://www.doi.org/10.1021/je3012452
Validation of the Vaporization Enthalpies of Some Simple Aliphatic Amides and Their Use in the Evaluation of the Vaporization Enthalpy of Valpromide and Valnoctamide:	

Legend

basg:	Gas basicity
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
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume