Hexanamide

Other names:	Caproic amide
	Hexamide
	Hexanoamide
	NCI-C02142
	NSC 8437
	caproamide
	capronamide
	hexylamide
	n-Caproamide
	n-Caproic amide
	n-hexanamide
Inchi:	InChI=1S/C6H13NO/c1-2-3-4-5-6(7)8/h2-5H2,1H3,(H2,7,8)
InchiKey:	ALBYIUDWACNRRB-UHFFFAOYSA-N
Formula:	C6H13NO
SMILES:	CCCCCC(N)=O
Mol. weight [g/mol]:	115.17
CAS:	628-02-4

Physical Properties

Property code	Value	Unit	Source
basg	854.00 ± 5.00	kJ/mol	NIST Webbook
basg	850.00 ± 6.00	kJ/mol	NIST Webbook
chs	-3796.00 ± 0.42	kJ/mol	NIST Webbook
chs	-3794.30 ± 0.75	kJ/mol	NIST Webbook
gf	-62.83	kJ/mol	Joback Method
hf	-245.96	kJ/mol	Joback Method
hfs	-423.00 ± 0.42	kJ/mol	NIST Webbook
hfus	16.70	kJ/mol	Heat Capacities and Enthalpies of Solid-Solid Transitions and Fusion of a Series of Eleven Primary Alkylamides by Differential Scanning Calorimetry
hsub	95.10 ± 0.40	kJ/mol	NIST Webbook
hsub	98.70 ± 1.70	kJ/mol	NIST Webbook
hsub	85.00 ± 4.00	kJ/mol	NIST Webbook
hvap	46.34	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method

logp	1.052		Crippen Method
mcvol	106.950	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
rinpol	1135.00		NIST Webbook
tb	463.08	K	Joback Method
tc	654.46	K	Joback Method
tf	372.40	K	Validation of the Vaporization Enthalpies of Some Simple Aliphatic Amides and Their Use in the Evaluation of the Vaporization Enthalpy of Valpromide and Valnoctamide
tf	373.80 ± 1.00	K	NIST Webbook
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.69	J/mol×K	463.08	Joback Method
cpg	239.44	J/mol×K	494.98	Joback Method
cpg	249.71	J/mol×K	526.87	Joback Method
cpg	259.51	J/mol×K	558.77	Joback Method
cpg	268.86	J/mol×K	590.67	Joback Method
cpg	277.77	J/mol×K	622.56	Joback Method
cpg	286.25	J/mol×K	654.46	Joback Method
hfust	16.70	kJ/mol	373.00	NIST Webbook
hfust	25.10	kJ/mol	374.00	NIST Webbook
hsubt	99.00 ± 2.00	kJ/mol	293.00	NIST Webbook
hsubt	95.00 ± 4.00	kJ/mol	353.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C628024&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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 Series of Primary Alkylamides by Differential Scanning Calorimetry:	https://www.doi.org/10.1021/je700662a
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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