Octanamide

Other names: caprylamide
Inchi: InChI=1S/C8H17NO/c1-2-3-4-5-6-7-8(9)10/h2-7H2,1H3,(H2,9,10)
InchiKey: LTHCSWBWNVGEFE-UHFFFAOYSA-N
Formula: C8H17NO
SMILES: CCCCCCCC(N)=O
Mol. weight [g/mol]: 143.23
CAS: 629-01-6

Physical Properties

Property code	Value	Unit	Source
chs	-5104.48 ± 0.84	kJ/mol	NIST Webbook
gf	-45.99	kJ/mol	Joback Method
hf	-287.24	kJ/mol	Joback Method
hfus	27.60	kJ/mol	Heat Capacities and Enthalpies of Solid-Solid Transitions and Fusion of a Series of Eleven Primary Alkylamides by Differential Scanning Calorimetry
hsub	110.00 ± 3.00	kJ/mol	NIST Webbook
hvap	50.79	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	1.832		Crippen Method
mcvol	135.130	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	1326.00		NIST Webbook
tb	508.84	K	Joback Method
tc	695.96	K	Joback Method
tf	381.90 ± 2.00	K	NIST Webbook
tf	378.65 ± 2.00	K	NIST Webbook
tf	378.80 ± 0.60	K	NIST Webbook
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	313.79	J/mol×K	508.84	Joback Method
cpg	326.61	J/mol×K	540.03	Joback Method
cpg	338.86	J/mol×K	571.21	Joback Method
cpg	350.55	J/mol×K	602.40	Joback Method
cpg	361.69	J/mol×K	633.59	Joback Method
cpg	372.30	J/mol×K	664.77	Joback Method
cpg	382.39	J/mol×K	695.96	Joback Method
hfust	27.60	kJ/mol	377.00	NIST Webbook
hsubt	110.50 ± 2.90	kJ/mol	349.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
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=C629016&Units=SI

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

vc: Critical Volume