

Heptanamide

Other names:	Enanthic acid amide Heptanamide (enantamide) enantamide heptamide
Inchi:	InChI=1S/C7H15NO/c1-2-3-4-5-6-7(8)9/h2-6H2,1H3,(H2,8,9)
InchiKey:	AEDIXYWIVPYNBI-UHFFFAOYSA-N
Formula:	C7H15NO
SMILES:	CCCCCCC(N)=O
Mol. weight [g/mol]:	129.20

Physical Properties

Property code	Value	Unit	Source
af	0.6208		Cheméo Relay (1.0)
gf	-54.41	kJ/mol	Joback Method
hf	-390.47	kJ/mol	Cheméo Relay (1.0)
hfus	20.68	kJ/mol	Joback Method
hvap	56.48	kJ/mol	Cheméo Relay (1.0)
ie	9.81	eV	Cheméo Relay (1.0)
log10ws	-1.94		Cheméo Relay (1.0)
logp	1.442		Crippen Method
mcvol	121.040	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
tb	479.09	K	Cheméo Relay (1.0)
tc	674.38	K	Cheméo Relay (1.0)
tf	369.00 ± 3.00	K	NIST Webbook
tf	368.60	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	369.80 ± 0.60	K	NIST Webbook
vc	0.460	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.23	J/mol×K	485.96	Joback Method
cpg	282.08	J/mol×K	517.50	Joback Method
cpg	293.39	J/mol×K	549.04	Joback Method
cpg	304.20	J/mol×K	580.59	Joback Method
cpg	314.49	J/mol×K	612.13	Joback Method
cpg	324.30	J/mol×K	643.67	Joback Method
cpg	333.64	J/mol×K	675.21	Joback Method
hsubt	99.60	kJ/mol	355.00	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
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
NIST Webbook	http://webbook.nist.gov/cgi/cbook.cgi?ID=C628626&Units=SI

Legend

af:	Acentric Factor
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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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

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