

N-amylglycine

Inchi:	InChI=1S/C7H15NO2/c1-2-3-4-5-6(8)7(9)10/h6H,2-5,8H2,1H3,(H,9,10)
InchiKey:	RDFMDVXONNIGBC-UHFFFAOYSA-N
Formula:	C7H15NO2
SMILES:	CCCCC(N)C(=O)O
Mol. weight [g/mol]:	145.20
CAS:	1115-90-8

Physical Properties

Property code	Value	Unit	Source
gf	-193.67	kJ/mol	Joback Method
hf	-424.11	kJ/mol	Joback Method
hfus	21.25	kJ/mol	Joback Method
hvap	64.85	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	0.979		Crippen Method
mvol	126.910	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
tb	577.70	K	Joback Method
tc	760.93	K	Joback Method
tf	347.66	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.47	J/molxK	577.70	Joback Method
cpg	330.79	J/molxK	608.24	Joback Method
cpg	340.62	J/molxK	638.78	Joback Method
cpg	349.98	J/molxK	669.31	Joback Method
cpg	358.87	J/molxK	699.85	Joback Method
cpg	367.32	J/molxK	730.39	Joback Method
cpg	375.33	J/molxK	760.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1115908&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/29-482-5/N-amylglycine.pdf>

Generated by Cheméo on 2024-04-26 14:19:25.212819031 +0000 UTC m=+16430414.133396343.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.