N-Acetyl-D-glucosamine

Other names:	2-Acetamido-2-deoxy-D-glucose
	2-Acetamido-2-deoxyglucose
	2-Acetamido-D-glucose
	2-acetylamino-2-deoxy-D-glucose
	Acetylglucosamine
	D-Glucose, 2-(acetylamino)-2-deoxy-
	D-Glucose, 2-acetamido-2-deoxy-
	N-((2R,3R,4S,5R)-3,4,5,6-tetrahydroxy-1-oxohexan-2-yl)acetamide
	N-Acetylglucosamine
	N-acetyl-«beta»-D-glucosamine
	NSC 524344
	d-N-Acetylglucosamine
Inchi:	InChI=1S/C8H15NO6/c1-4(12)9-5(2-10)7(14)8(15)6(13)3-11/h2,5-8,11,13-15H,3H2,1H3,
InchiKey:	MBLBDJOUHNCFQT-UHFFFAOYSA-N
Formula:	C8H15NO6
SMILES:	CC(O)=NC(C=O)C(O)C(O)C(O)CO
Mol. weight [g/mol]:	221.21
CAS:	7512-17-6

Physical Properties

Property code	Value	Unit	Source
hf	-1003.87	kJ/mol	Joback Method
hvap	125.36	kJ/mol	Joback Method
log10ws	1.06		Crippen Method
logp	-2.395		Crippen Method
mcvol	160.180	ml/mol	McGowan Method
pc	4328.25	kPa	Joback Method
tb	966.80	K	Joback Method
tc	1189.18	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cps	269.80	J/mol×K	288.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	276.40	J/mol×K	293.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	276.90	J/mol×K	298.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	278.00	J/mol×K	303.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	283.30	J/mol×K	308.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	281.00	J/mol×K	313.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	281.40	J/mol×K	318.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	292.70	J/mol×K	323.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	293.10	J/mol×K	328.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides

cps	299.40	J/mol×K	333.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	303.80	J/mol×K	338.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	308.70	J/mol×K	343.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	319.70	J/mol×K	348.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	325.20	J/mol×K	353.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides
cps	332.00	J/mol×K	358.15	Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7512176&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Apparent molar volumes and apparent molar heat capacities of aqueous N-acetyl-D-glucosamine at temperatures from 278.15 K to 393.15 K and of aqueous N-methylacetamide at temperatures from 278.15 K to 393.15 K at the pressure 0.35 MPa:	https://www.doi.org/10.1016/j.jct.2006.04.007
Temperature dependence of the heat capacities in the solid state of 18 mono-, di-, and poly-saccharides:	https://www.doi.org/10.1016/j.jct.2008.08.007
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature