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)N[C@@H]1[C@H](O)[C@@H](O)[C@@H](CO)O[C@H]1O
Mol. weight [g/mol]:	221.21

Physical Properties

Property code	Value	Unit	Source
hfus	43.62	kJ/mol	Joback Method
logp	-3.078		Crippen Method
mcvol	153.620	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.44	J/mol×K	883.02	Joback Method
cpg	545.94	J/mol×K	916.08	Joback Method
cpg	553.63	J/mol×K	949.13	Joback Method
cpg	560.51	J/mol×K	982.19	Joback Method
cpg	566.58	J/mol×K	1015.24	Joback Method
cpg	571.84	J/mol×K	1048.30	Joback Method
cpg	576.29	J/mol×K	1081.35	Joback Method

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

Cheméo Relay (1.0, beta):

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C10036643
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Apparent molar volumes and apparent molar heat capacities of aqueous N-acetyl-D-glucosamine 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 monor-, di-, and poly saccherides:	https://www.doi.org/10.1016/j.jct.2008.08.007

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume