2-Acetamido-2-deoxy-«alpha»-D-glucopyranose

Other names:	«alpha»-D-Glucopyranose, 2-(acetylamino)-2-deoxy- «alpha»-D-glucopyranoside, 2-acetamido-2-deoxy-, N-Acetyl-«alpha»-D-glucosamine Glucopyranose, 2-acetamido-2-deoxy-, «alpha»-D- Alpha,d-glucopyranoside, 2-acetamido-2-deoxy-,
Inchi:	InChI=1S/C8H15NO6/c1-3(11)9-5-7(13)6(12)4(2-10)15-8(5)14/h4-8,10,12-14H,2H2,1H3,
InchiKey:	OVRNDRQMDRJTHS-UHFFFAOYSA-N
Formula:	C8H15NO6
SMILES:	CC(=O)NC1C(O)OC(CO)C(O)C1O
Mol. weight [g/mol]:	221.21
CAS:	10036-64-3

Physical Properties

Property code	Value	Unit	Source
gf	-662.84	kJ/mol	Joback Method
hf	-1035.52	kJ/mol	Joback Method
hfus	43.62	kJ/mol	Joback Method
hvap	117.00	kJ/mol	Joback Method
log10ws	0.77		Crippen Method
logp	-3.078		Crippen Method
mcvol	153.620	ml/mol	McGowan Method
pc	4577.74	kPa	Joback Method
tb	883.02	K	Joback Method
tc	1081.35	K	Joback Method
tf	542.78	K	Joback Method
vc	0.550	m3/kmol	Joback 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

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10036643&Units=SI

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
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
tf:	Normal melting (fusion) point
vc:	Critical Volume