N-Acetyl-D-glucosamine, aldononitrile, tetraacetate

Inchi: InChI=1S/C16H22N2O9/c1-8(19)18-13(6-17)15(26-11(4)22)16(27-12(5)23)14(25-10(3)21

InchiKey: MMTPGHDGDMHPRG-UHFFFAOYSA-N

Formula: C16H22N2O9

SMILES: CC(=O)NC(C#N)C(OC(C)=O)C(OC(C)=O)C(COC(C)=O)OC(C)=O

Mol. weight [g/mol]: 386.35

Physical Properties

Property code	Value	Unit	Source
gf	-767.95	kJ/mol	Joback Method
hf	-1268.12	kJ/mol	Joback Method
hfus	42.46	kJ/mol	Joback Method
hvap	109.94	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	-0.627		Crippen Method
mcvol	278.990	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	2080.50		NIST Webbook
rinpol	2080.50		NIST Webbook
tb	1075.00	K	Joback Method
tc	1316.23	K	Joback Method
tf	666.30	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.88	J/mol×K	1075.00	Joback Method
cpg	898.85	J/mol×K	1115.20	Joback Method
cpg	901.82	J/mol×K	1155.41	Joback Method
cpg	902.76	J/mol×K	1195.61	Joback Method
cpg	901.64	J/mol×K	1235.82	Joback Method
cpg	898.43	J/mol×K	1276.02	Joback Method
cpg	893.09	J/mol×K	1316.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380428&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume