«alpha»-D-Glucopyranose, pentaacetate

Other names: Glucopyranose, pentaacetate, «alpha»-D-
«alpha»-D-Glucose pentaacetate
Pentaacetyl-«alpha»-D-glucose
D-«alpha»-Glucose pentaacetate
D-alpha-glucose pentaacetate
Alpha-d-glucose, pentaacetate

Inchi: InChI=1S/C16H22O11/c1-7(17)22-6-12-13(23-8(2)18)14(24-9(3)19)15(25-10(4)20)16(27

InchiKey: LPTITAGPBXDDGR-ARKGTOAJSA-N

Formula: C16H22O11

SMILES: CC(=O)OCC1OC(OC(C)=O)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O

Mol. weight [g/mol]: 390.34

CAS: 604-68-2

Physical Properties

Property code	Value	Unit	Source
gf	-1178.27	kJ/mol	Joback Method
hf	-1756.61	kJ/mol	Joback Method
hfus	55.23	kJ/mol	Joback Method
hvap	100.69	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	-0.367		Crippen Method
mcvol	268.510	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	2257.00		NIST Webbook
rinpol	2257.00		NIST Webbook
tb	974.75	K	Joback Method
tc	1196.79	K	Joback Method
tf	647.87	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.09	J/mol×K	974.75	Joback Method

cpg	916.30	J/mol×K	1011.76	Joback Method
cpg	923.29	J/mol×K	1048.76	Joback Method
cpg	927.99	J/mol×K	1085.77	Joback Method
cpg	930.33	J/mol×K	1122.77	Joback Method
cpg	930.22	J/mol×K	1159.78	Joback Method
cpg	927.59	J/mol×K	1196.79	Joback Method
dvisc	0.0004318	Pa×s	647.87	Joback Method
dvisc	0.0003009	Pa×s	702.35	Joback Method
dvisc	0.0002208	Pa×s	756.83	Joback Method
dvisc	0.0001689	Pa×s	811.31	Joback Method
dvisc	0.0001337	Pa×s	865.79	Joback Method
dvisc	0.0001087	Pa×s	920.27	Joback Method
dvisc	0.0000905	Pa×s	974.75	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=C604682&Units=SI

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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