«beta»-D-Glucopyranose pentaacetate

Other names:	Acetyl 2,3,4,6-tetra-O-acetyl-«beta»-D-glucopyranoside
	Glucopyranose, pentaacetate, «beta»-D-
	«beta»-D-Glucose pentaacetate
	Penta-O-acetyl-«beta»-D-glucopyranose
	Pentaacetyl-«beta»-D-glucopyranose
	Pentaacetyl-«beta»-D-glucose
	1,2,3,4,6-Penta-O-acetyl-«beta»-D-glucopyranose
	«beta»-D-Glucopyranosyl pentaacetate
	1,2,3,4,6-Penta-O-acetylglucopyranose, «beta»-D-
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-QMHWVQJVSA-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:	604-69-3

Physical Properties

Property code	Value	Unit	Source
chs	-7207.70 ± 1.90	kJ/mol	NIST Webbook
gf	-1178.27	kJ/mol	Joback Method
hf	-1756.61	kJ/mol	Joback Method
hfs	-2232.60 ± 2.00	kJ/mol	NIST Webbook
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
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: 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=C604693&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase 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