«beta»-D-Glucopyranose, 1,6-anhydro-

Other names:	1,6-Anhydro-beta-D-glucopyranose
	1,6-Anhydro-«beta»-D-glucopyranose
	1,6-Anhydro-«beta»-D-glucopyranose (levoglucosan)
	1,6-anhydro-.beta.-D-glucopyranose
	1,6-anhydro-«beta»-D-glucose
	1,6-dihydro-.beta.-D-glucopyranose
	Anhydro-d-mannosan
	levoglucosan
Inchi:	InChI=1S/C6H10O5/c7-3-2-1-10-6(11-2)5(9)4(3)8/h2-9H,1H2
InchiKey:	TWNIBLMWSKIRAT-UHFFFAOYSA-N
Formula:	C6H10O5
SMILES:	OC1C2COC(O2)C(O)C1O
Mol. weight [g/mol]:	162.14
CAS:	498-07-7

Physical Properties

Property code	Value	Unit	Source
chs	-2832.00 ± 0.80	kJ/mol	NIST Webbook
chs	-2875.10	kJ/mol	NIST Webbook
gf	-508.89	kJ/mol	Joback Method
hf	-815.60	kJ/mol	Joback Method
hfus	34.80	kJ/mol	Joback Method
hvap	87.25	kJ/mol	Joback Method
log10ws	0.86		Crippen Method
logp	-2.176		Crippen Method
mcvol	103.030	ml/mol	McGowan Method
pc	5695.98	kPa	Joback Method
rinpol	1491.10		NIST Webbook
tb	675.13	K	Joback Method
tc	856.72	K	Joback Method
tf	409.10	K	Joback Method
tt	384.90	K	Levoglucosan: A Calorimetric, Thermodynamic, Spectroscopic, and Computational Investigation
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.91	J/mol×K	826.45	Joback Method
cpg	359.28	J/mol×K	765.92	Joback Method
cpg	351.27	J/mol×K	735.66	Joback Method
cpg	342.77	J/mol×K	705.39	Joback Method
cpg	333.75	J/mol×K	675.13	Joback Method
cpg	366.82	J/mol×K	796.19	Joback Method
cpg	380.58	J/mol×K	856.72	Joback Method
dvisc	0.0056868	Pa×s	409.10	Joback Method
dvisc	0.0000403	Pa×s	675.13	Joback Method
dvisc	0.0000687	Pa×s	630.79	Joback Method
dvisc	0.0001273	Pa×s	586.45	Joback Method
dvisc	0.0002606	Pa×s	542.12	Joback Method
dvisc	0.0006065	Pa×s	497.78	Joback Method
dvisc	0.0016646	Pa×s	453.44	Joback Method
hsubt	125.10 ± 1.00	kJ/mol	365.00	NIST Webbook
hsubt	100.30 ± 5.90	kJ/mol	395.50	NIST Webbook
hvapt	92.20	kJ/mol	498.00	NIST Webbook

Sources

Levoglucosan: A Calorimetric, Thermodynamic, Spectroscopic, and Computational Investigation: https://www.doi.org/10.1021/je400207t

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=C498077&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tt:	Triple Point Temperature
vc:	Critical Volume