«alpha»-D-Glucose

Other names: «alpha»-D-Glucopyranose
Inchi: InChI=1S/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6+/m0/s1
InchiKey: WQZGKKKJIJFFOK-MDMQIMBFSA-N
Formula: C6H12O6
SMILES: OCC1OC(O)C(O)C(O)C1O
Mol. weight [g/mol]: 180.16
CAS: 492-62-6

Physical Properties

Property code	Value	Unit	Source
chs	-2805.00 ± 1.30	kJ/mol	NIST Webbook
gf	-776.97	kJ/mol	Joback Method
hf	-1087.36	kJ/mol	Joback Method
hfus	35.83	kJ/mol	Joback Method
hvap	116.05	kJ/mol	Joback Method
log10ws	1.31		Crippen Method
logp	-3.221		Crippen Method
mcvol	119.760	ml/mol	McGowan Method
pc	6200.01	kPa	Joback Method
ss	209.19	J/mol×K	NIST Webbook
tb	825.40	K	Joback Method
tc	1011.14	K	Joback Method
tf	478.47	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.13	J/mol×K	825.40	Joback Method
cpg	425.76	J/mol×K	856.36	Joback Method
cpg	432.81	J/mol×K	887.31	Joback Method
cpg	439.26	J/mol×K	918.27	Joback Method
cpg	445.12	J/mol×K	949.22	Joback Method
cpg	450.39	J/mol×K	980.18	Joback Method

cpg	455.08	J/mol×K	1011.14	Joback Method
cps	229.30	J/mol×K	300.00	NIST Webbook
cps	221.00	J/mol×K	300.00	NIST Webbook
cps	219.79	J/mol×K	298.15	NIST Webbook
cps	224.00	J/mol×K	303.00	NIST Webbook
cps	218.80	J/mol×K	298.15	NIST Webbook
cps	218.00	J/mol×K	298.00	NIST Webbook
cps	219.19	J/mol×K	298.15	NIST Webbook
cps	211.30	J/mol×K	298.10	NIST Webbook
cps	220.90	J/mol×K	298.00	NIST Webbook
dvisc	0.0004404	Pa×s	478.47	Joback Method
dvisc	0.0000602	Pa×s	536.29	Joback Method
dvisc	0.0000121	Pa×s	594.11	Joback Method
dvisc	0.0000032	Pa×s	651.93	Joback Method
dvisc	0.0000011	Pa×s	709.76	Joback Method
dvisc	0.0000004	Pa×s	767.58	Joback Method
dvisc	0.0000002	Pa×s	825.40	Joback Method
hfust	31.42	kJ/mol	414.00	NIST Webbook
hfust	31.42	kJ/mol	414.00	NIST Webbook
hfust	34.30	kJ/mol	423.20	NIST Webbook
sfust	75.90	J/mol×K	414.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C492626&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase 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

hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume