Fructose

Inchi: InChI=1S/C6H12O6/c7-2-6(11)5(10)4(9)3(8)1-12-6/h3-5,7-11H,1-2H2/t3-,4-,5+,6-/m1/s1
InchiKey: LKDRXBCSQODPBY-ARQDHWQXSA-N
Formula: C6H12O6
SMILES: OCC1(O)OCC(O)C(O)C1O
Mol. weight [g/mol]: 180.16
CAS: 7660-25-5

Physical Properties

Property code	Value	Unit	Source
gf	-774.75	kJ/mol	Joback Method
hf	-1051.78	kJ/mol	Joback Method
hfus	28.46	kJ/mol	Joback Method
hvap	115.21	kJ/mol	Joback Method
log10ws	1.42		Crippen Method
logp	-3.220		Crippen Method
mcvol	119.760	ml/mol	McGowan Method
pc	7037.97	kPa	Joback Method
tb	830.31	K	Joback Method
tc	1017.85	K	Joback Method
tf	506.61	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.17	J/mol×K	830.31	Joback Method
cpg	417.53	J/mol×K	861.57	Joback Method
cpg	425.78	J/mol×K	892.82	Joback Method
cpg	434.00	J/mol×K	924.08	Joback Method
cpg	442.23	J/mol×K	955.34	Joback Method
cpg	450.53	J/mol×K	986.59	Joback Method
cpg	458.97	J/mol×K	1017.85	Joback Method
cps	201.00	J/mol×K	300.00	NIST Webbook
cps	230.50	J/mol×K	300.00	NIST Webbook

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=C7660255&Units=SI

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume