

Fructose

Other names:	«beta»-d-Fructose D-Fructose Levulose
Inchi:	InChI=1S/C6H12O6/c7-1-3(9)5(11)6(12)4(10)2-8/h3,5-9,11-12H,1-2H2/t3-,5-,6-/m1/s1
InchiKey:	BJHIKXHVCXFQLS-UYFOZJQFSA-N
Formula:	C6H12O6
SMILES:	O=C(CO)C(O)C(O)C(O)CO
Mol. weight [g/mol]:	180.16
CAS:	57-48-7

Physical Properties

Property code	Value	Unit	Source
chs	-2810.40 ± 0.30	kJ/mol	NIST Webbook
gf	-820.70	kJ/mol	Joback Method
hf	-1056.74	kJ/mol	Joback Method
hfs	-1265.60 ± 0.46	kJ/mol	NIST Webbook
hfus	22.77	kJ/mol	Joback Method
hvap	117.93	kJ/mol	Joback Method
log10ws	1.73		Crippen Method
logp	-3.377		Crippen Method
mcvol	126.320	ml/mol	McGowan Method
pc	6430.83	kPa	Joback Method
tb	850.13	K	Joback Method
tc	1041.01	K	Joback Method
tf	466.41	K	Joback Method
vc	0.455	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.42	J/mol×K	850.13	Joback Method
cpg	414.12	J/mol×K	1009.20	Joback Method
cpg	409.65	J/mol×K	977.39	Joback Method
cpg	404.87	J/mol×K	945.57	Joback Method

cpg	399.74	J/molxK	913.76	Joback Method
cpg	394.27	J/molxK	881.94	Joback Method
cpg	418.30	J/molxK	1041.01	Joback Method
dvisc	4.5130364e-08	Paxs	850.13	Joback Method
dvisc	0.0000001	Paxs	786.18	Joback Method
dvisc	0.0000004	Paxs	722.22	Joback Method
dvisc	0.0000013	Paxs	658.27	Joback Method
dvisc	0.0000066	Paxs	594.32	Joback Method
dvisc	0.0000482	Paxs	530.36	Joback Method
dvisc	0.0006126	Paxs	466.41	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=C57487&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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