

«beta»-D-Glucopyranoside, methyl

Other names:	Glucopyranoside, methyl, «beta»-D-Methyl «beta»-D-glucopyranoside Methyl «beta»-D-glucoside 1-O-Methyl-«beta»-D-glucopyranoside «beta»-d-Methylglucopyranoside «beta»-Methyl-(d)-glucoside
Inchi:	InChI=1S/C7H14O6/c1-12-7-6(11)5(10)4(9)3(2-8)13-7/h3-11H,2H2,1H3/t3-,4-,5+,6-,7-/m
InchiKey:	HOVAGTYPDGVJG-ZYNSJIGGSA-N
Formula:	C7H14O6
SMILES:	COC1OC(CO)C(O)C(O)C1O
Mol. weight [g/mol]:	194.18
CAS:	709-50-2

Physical Properties

Property code	Value	Unit	Source
chs	-3517.90 ± 0.42	kJ/mol	NIST Webbook
gf	-736.73	kJ/mol	Joback Method
hf	-1087.99	kJ/mol	Joback Method
hfus	35.52	kJ/mol	Joback Method
hvap	104.00	kJ/mol	Joback Method
log10ws	1.07		Crippen Method
logp	-2.567		Crippen Method
mcvol	133.850	ml/mol	McGowan Method
pc	4596.38	kPa	Joback Method
tb	778.52	K	Joback Method
tc	958.16	K	Joback Method
tf	451.15	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.93	J/mol×K	778.52	Joback Method
cpg	460.26	J/mol×K	808.46	Joback Method

cpg	468.98	J/mol×K	838.40	Joback Method
cpg	477.06	J/mol×K	868.34	Joback Method
cpg	484.50	J/mol×K	898.28	Joback Method
cpg	491.30	J/mol×K	928.22	Joback Method
cpg	497.43	J/mol×K	958.16	Joback Method
dvisc	0.0009928	Pa×s	451.15	Joback Method
dvisc	0.0001720	Pa×s	505.71	Joback Method
dvisc	0.0000419	Pa×s	560.27	Joback Method
dvisc	0.0000131	Pa×s	614.84	Joback Method
dvisc	0.0000050	Pa×s	669.40	Joback Method
dvisc	0.0000022	Pa×s	723.96	Joback Method
dvisc	0.0000011	Pa×s	778.52	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=C709502&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
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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