

«alpha»-D-Glucopyranoside, methyl

Other names:	Glucopyranoside, methyl, «alpha»-D- «alpha»-Methylglucoside Methyl «alpha»-D-glucopyranoside Methyl «alpha»-D-glucoside «alpha»-d-Methylglucopyranoside «alpha»-Methyl D-glucose ether «alpha»-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:	HOVAGTYPODGVJG-NEVCITSRSA-N
Formula:	C7H14O6
SMILES:	COC1OC(CO)C(O)C(O)C1O
Mol. weight [g/mol]:	194.18
CAS:	97-30-3

Physical Properties

Property code	Value	Unit	Source
chs	-3528.50	kJ/mol	NIST Webbook
chs	-3522.10 ± 0.84	kJ/mol	NIST Webbook
chs	-3529.22 ± 0.19	kJ/mol	NIST Webbook
gf	-736.73	kJ/mol	Joback Method
hf	-1087.99	kJ/mol	Joback Method
hfs	-1228.20	kJ/mol	NIST Webbook
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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.93	J/molxK	778.52	Joback Method
cpg	460.26	J/molxK	808.46	Joback Method
cpg	468.98	J/molxK	838.40	Joback Method
cpg	477.06	J/molxK	868.34	Joback Method
cpg	484.50	J/molxK	898.28	Joback Method
cpg	491.30	J/molxK	928.22	Joback Method
cpg	497.43	J/molxK	958.16	Joback Method
dvisc	0.0009928	Paxs	451.15	Joback Method
dvisc	0.0001720	Paxs	505.71	Joback Method
dvisc	0.0000419	Paxs	560.27	Joback Method
dvisc	0.0000131	Paxs	614.84	Joback Method
dvisc	0.0000050	Paxs	669.40	Joback Method
dvisc	0.0000022	Paxs	723.96	Joback Method
dvisc	0.0000011	Paxs	778.52	Joback Method

Sources

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=C97303&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
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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