

D-gulose

Inchi:	InChI=1S/C6H12O6/c7-1-3(9)5(11)6(12)4(10)2-8/h1,3-6,8-12H,2H2/t3-,4+,5-,6-/m1/s1
InchiKey:	GZCGUPFRVQAUUE-JGWLITMVSA-N
Formula:	C6H12O6
SMILES:	O=CC(O)C(O)C(O)C(O)CO
Mol. weight [g/mol]:	180.16
CAS:	4205-23-6

Physical Properties

Property code	Value	Unit	Source
chs	-2817.30	kJ/mol	NIST Webbook
gf	-793.74	kJ/mol	Joback Method
hf	-1035.02	kJ/mol	Joback Method
hfus	19.93	kJ/mol	Joback Method
hvap	117.51	kJ/mol	Joback Method
log10ws	1.62		Crippen Method
logp	-3.379		Crippen Method
mcvol	126.320	ml/mol	McGowan Method
pc	6631.37	kPa	Joback Method
tb	844.48	K	Joback Method
tc	1034.02	K	Joback Method
tf	443.48	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.04	J/mol×K	844.48	Joback Method
cpg	415.49	J/mol×K	1002.43	Joback Method
cpg	411.06	J/mol×K	970.84	Joback Method
cpg	406.32	J/mol×K	939.25	Joback Method
cpg	401.25	J/mol×K	907.66	Joback Method
cpg	395.83	J/mol×K	876.07	Joback Method
cpg	419.64	J/mol×K	1034.02	Joback Method
dvisc	4.8974616e-08	Pa×s	844.48	Joback Method

dvisc	0.0000001	Pa×s	777.65	Joback Method
dvisc	0.0000004	Pa×s	710.81	Joback Method
dvisc	0.0000018	Pa×s	643.98	Joback Method
dvisc	0.0000107	Pa×s	577.15	Joback Method
dvisc	0.0000991	Pa×s	510.31	Joback Method
dvisc	0.0017994	Pa×s	443.48	Joback Method

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=C4205236&Units=SI

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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