

«alpha», «beta»-Gluco-octonic acid lactone

Other names:	D-erythro-L-talo-Octonic acid, «gamma»-lactone D-erythro-L-talo-Octonic acid, Å«gammaÅ»-lactone D-erythro-L-talo-octono-1,4-lactone alpha, beta-Glucooctanoic gamma-lactone
Inchi:	InChI=1S/C8H14O8/c9-1-2(10)3(11)4(12)7-5(13)6(14)8(15)16-7/h2-7,9-14H,1H2
InchiKey:	NUYDBDGECBIUPJ-UHFFFAOYSA-N
Formula:	C8H14O8
SMILES:	O=C1OC(C(O)C(O)C(O)CO)C(O)C1O
Mol. weight [g/mol]:	238.19
CAS:	6968-62-3

Physical Properties

Property code	Value	Unit	Source
gf	-999.34	kJ/mol	Joback Method
hf	-1387.57	kJ/mol	Joback Method
hfus	34.00	kJ/mol	Joback Method
hvap	140.71	kJ/mol	Joback Method
log10ws	1.82		Crippen Method
logp	-4.291		Crippen Method
mcvol	155.380	ml/mol	McGowan Method
pc	6200.01	kPa	Joback Method
tb	1034.91	K	Joback Method
tc	1284.36	K	Joback Method
tf	597.05	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.70	J/molxK	1034.91	Joback Method
cpg	572.41	J/molxK	1076.48	Joback Method
cpg	576.90	J/molxK	1118.06	Joback Method
cpg	580.17	J/molxK	1159.63	Joback Method
cpg	582.22	J/molxK	1201.21	Joback Method

cpg	583.06	J/mol×K	1242.78	Joback Method
cpg	582.67	J/mol×K	1284.36	Joback Method
cps	245.34	J/mol×K	298.15	Enthalpies of combustion and formation of a-D-glucoheptono-1,4-lactone and a,b-glucooctanoic-1,4-lactone

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6968623&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Enthalpies of combustion and formation of a-D-glucoheptono-1,4-lactone and a,b-glucooctanoic-1,4-lactone:	https://www.doi.org/10.1016/j.jct.2007.12.007
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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