ALPHA-D-GLUCOHEPTONIC ACID GAMMA-LACTONE

Other names: 3,4-dihydroxy-5-(1,2,3-trihydroxypropyl)oxolan-2-one
D-glycero-D-gulo-heptono-1,4-lactone
Inchi: InChI=1S/C7H12O7/c8-1-2(9)3(10)6-4(11)5(12)7(13)14-6/h2-6,8-12H,1H2
InchiKey: VIVCRCODGMFTFY-UHFFFAOYSA-N
Formula: C7H12O7
SMILES: O=C1OC(C(O)C(O)CO)C(O)C1O
Mol. weight [g/mol]: 208.17

Physical Properties

Property code	Value	Unit	Source
chs	-2981.90 ± 4.10	kJ/mol	NIST Webbook
hfus	30.85	kJ/mol	Joback Method
log10ws	0.39		Aqueous Solubility Prediction Method
logp	-3.652		Crippen Method
mcvol	135.420	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.78	J/mol×K	920.29	Joback Method
cpg	482.50	J/mol×K	954.74	Joback Method
cpg	488.45	J/mol×K	989.19	Joback Method
cpg	493.62	J/mol×K	1023.64	Joback Method
cpg	498.01	J/mol×K	1058.09	Joback Method
cpg	501.60	J/mol×K	1092.53	Joback Method
cpg	504.40	J/mol×K	1126.98	Joback Method

Sources

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89678&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume