

D-glycero-D-gulo-Heptonic 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
CAS:	89-67-8

Physical Properties

Property code	Value	Unit	Source
chs	-2981.90 ± 4.10	kJ/mol	NIST Webbook
gf	-868.50	kJ/mol	Joback Method
hf	-1209.42	kJ/mol	Joback Method
hfus	30.85	kJ/mol	Joback Method
hvap	122.19	kJ/mol	Joback Method
log10ws	0.39		Aqueous Solubility Prediction Method
logp	-3.652		Crippen Method
mcvol	135.420	ml/mol	McGowan Method
pc	6161.14	kPa	Joback Method
tb	920.29	K	Joback Method
tc	1126.98	K	Joback Method
tf	539.96	K	Joback Method
vc	0.477	m ³ /kmol	Joback 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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89678&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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

Latest version available from:

<https://www.cheméo.com/cid/60-134-6/D-glycero-D-gulo-Heptonic-acid-gamma-lactone.pdf>

Generated by Cheméo on 2024-04-18 03:45:27.004815835 +0000 UTC m=+15701175.925393151.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.