

D-glucaro-3,6-lactone

Other names:	D-Glucaric acid 3,6-lactone
Inchi:	InChI=1S/C6H8O7/c7-1-2(8)6(12)13-4(1)3(9)5(10)11/h1-4,7-9H,(H,10,11)/t1-,2-,3-,4+/m1
InchiKey:	XECPAIJNBXCBOB-AJSXGEPRSA-N
Formula:	C6H8O7
SMILES:	O=C1OC(C(O)C(=O)O)C(O)C1O
Mol. weight [g/mol]:	192.12
CAS:	2782-04-9

Physical Properties

Property code	Value	Unit	Source
chs	-2066.80 ± 3.00	kJ/mol	NIST Webbook
gf	-866.58	kJ/mol	Joback Method
hf	-1143.85	kJ/mol	Joback Method
hfus	29.29	kJ/mol	Joback Method
hvap	110.42	kJ/mol	Joback Method
log10ws	1.57		Crippen Method
logp	-2.921		Crippen Method
mcvol	117.030	ml/mol	McGowan Method
pc	6774.04	kPa	Joback Method
tb	859.54	K	Joback Method
tc	1056.51	K	Joback Method
tf	532.80	K	Joback Method
vc	0.414	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.30	J/mol×K	859.54	Joback Method
cpg	392.53	J/mol×K	892.37	Joback Method
cpg	398.11	J/mol×K	925.20	Joback Method
cpg	403.04	J/mol×K	958.02	Joback Method
cpg	407.31	J/mol×K	990.85	Joback Method
cpg	410.90	J/mol×K	1023.68	Joback Method
cpg	413.82	J/mol×K	1056.51	Joback Method

Sources

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=C2782049&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

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