

Gluconic acid «delta»-lactone

Inchi:	InChI=1S/C6H10O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-5,7-10H,1H2
InchiKey:	PHOQVHQSTUBQQK-UHFFFAOYSA-N
Formula:	C6H10O6
SMILES:	O=C1OC(CO)C(O)C(O)C1O
Mol. weight [g/mol]:	178.14

Physical Properties

Property code	Value	Unit	Source
gf	-755.03	kJ/mol	Joback Method
hf	-1052.49	kJ/mol	Joback Method
hfus	30.19	kJ/mol	Joback Method
hvap	103.92	kJ/mol	Joback Method
log10ws	1.41		Crippen Method
logp	-3.013		Crippen Method
mcvol	115.460	ml/mol	McGowan Method
pc	5972.16	kPa	Joback Method
tb	805.71	K	Joback Method
tc	994.24	K	Joback Method
tf	490.11	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.22	J/molxK	805.71	Joback Method
cpg	397.10	J/molxK	837.13	Joback Method
cpg	404.34	J/molxK	868.55	Joback Method
cpg	410.92	J/molxK	899.98	Joback Method
cpg	416.82	J/molxK	931.40	Joback Method
cpg	422.03	J/molxK	962.82	Joback Method
cpg	426.52	J/molxK	994.24	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=B6001588&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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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