

I-Gulonic acid, «gamma»-lactone

Other names:	(l)-gulono-1,4-lactone
Inchi:	InChI=1S/C6H10O6/c7-1-2(8)5-3(9)4(10)6(11)12-5/h2-5,7-10H,1H2
InchiKey:	SXZYCXMUPBBULW-UHFFFAOYSA-N
Formula:	C6H10O6
SMILES:	O=C1OC(C(O)CO)C(O)C1O
Mol. weight [g/mol]:	178.14
CAS:	1128-23-0

Physical Properties

Property code	Value	Unit	Source
gf	-737.66	kJ/mol	Joback Method
hf	-1031.27	kJ/mol	Joback Method
hfus	27.69	kJ/mol	Joback Method
hvap	103.67	kJ/mol	Joback Method
log10ws	1.41		Crippen Method
logp	-3.013		Crippen Method
mcvol	115.460	ml/mol	McGowan Method
pc	6122.63	kPa	Joback Method
tb	805.67	K	Joback Method
tc	993.39	K	Joback Method
tf	482.87	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.51	J/mol×K	805.67	Joback Method
cpg	389.93	J/mol×K	836.96	Joback Method
cpg	396.79	J/mol×K	868.24	Joback Method
cpg	403.08	J/mol×K	899.53	Joback Method
cpg	408.80	J/mol×K	930.82	Joback Method
cpg	413.93	J/mol×K	962.10	Joback Method
cpg	418.48	J/mol×K	993.39	Joback Method
hfust	41.50	kJ/mol	459.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1128230&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hfust:	Enthalpy of fusion at a given temperature
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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