«GAMMA»-glucuronolactone

Inchi: InChI=1S/C6H8O6/c7-1-2(8)5-3(9)4(10)6(11)12-5/h1-5,8-10H
InchiKey: UYUXSRADSPPKRZ-UHFFFAOYSA-N
Formula: C6H8O6
SMILES: O=CC(O)C1OC(=O)C(O)C1O
Mol. weight [g/mol]: 176.12

Physical Properties

Property code	Value	Unit	Source
gf	-700.36	kJ/mol	Joback Method
hf	-964.62	kJ/mol	Joback Method
hfus	25.89	kJ/mol	Joback Method
hvap	93.72	kJ/mol	Joback Method
log10ws	1.39		Crippen Method
logp	-2.807		Crippen Method
mcvol	111.160	ml/mol	McGowan Method
pc	5953.74	kPa	Joback Method
tb	762.15	K	Joback Method
tc	953.14	K	Joback Method
tf	464.05	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.50	J/mol×K	762.15	Joback Method
cpg	356.09	J/mol×K	793.98	Joback Method
cpg	363.13	J/mol×K	825.81	Joback Method
cpg	369.61	J/mol×K	857.65	Joback Method
cpg	375.52	J/mol×K	889.48	Joback Method
cpg	380.85	J/mol×K	921.31	Joback Method
cpg	385.59	J/mol×K	953.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6001587&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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