2(S)-hydroxy-«gamma»-butyrolactone

Inchi: InChI=1S/C4H6O3/c5-3-1-2-7-4(3)6/h3,5H,1-2H2/t3-/m1/s1
InchiKey: FWIBCWKHNZBDLS-GSVOUGTGSA-N
Formula: C4H6O3
SMILES: O=C1OCCC1O
Mol. weight [g/mol]: 102.09

Physical Properties

Property code	Value	Unit	Source
gf	-326.18	kJ/mol	Joback Method
hf	-487.34	kJ/mol	Joback Method
hfus	11.63	kJ/mol	Joback Method
hvap	50.19	kJ/mol	Joback Method
log10ws	0.37		Crippen Method
logp	-0.706		Crippen Method
mcvol	69.670	ml/mol	McGowan Method
pc	5880.91	kPa	Joback Method
ripol	1692.00		NIST Webbook
ripol	1692.00		NIST Webbook
tb	493.15	K	Joback Method
tc	701.93	K	Joback Method
tf	301.35	K	Joback Method
vc	0.247	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.21	J/mol×K	493.15	Joback Method
cpg	166.07	J/mol×K	527.95	Joback Method
cpg	174.55	J/mol×K	562.74	Joback Method
cpg	182.66	J/mol×K	597.54	Joback Method
cpg	190.39	J/mol×K	632.34	Joback Method
cpg	197.73	J/mol×K	667.13	Joback Method
cpg	204.66	J/mol×K	701.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R519070&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume