5-Methyl-4-hydroxy-3(2H)-furanone

Inchi: InChI=1S/C5H6O3/c1-3-5(7)4(6)2-8-3/h7H,2H2,1H3
InchiKey: DLVYTANECMRFGX-UHFFFAOYSA-N
Formula: C5H6O3
SMILES: CC1=C(O)C(=O)CO1
Mol. weight [g/mol]: 114.10

Physical Properties

Property code	Value	Unit	Source
gf	-299.35	kJ/mol	Joback Method
hf	-452.80	kJ/mol	Joback Method
hfus	13.59	kJ/mol	Joback Method
hvap	54.34	kJ/mol	Joback Method
log10ws	-0.35		Crippen Method
logp	0.375		Crippen Method
mcvol	79.460	ml/mol	McGowan Method
pc	5398.63	kPa	Joback Method
ripol	2069.00		NIST Webbook
tb	529.82	K	Joback Method
tc	739.97	K	Joback Method
tf	342.66	K	Joback Method
vc	0.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.29	J/mol×K	529.82	Joback Method
cpg	185.19	J/mol×K	564.85	Joback Method
cpg	192.77	J/mol×K	599.87	Joback Method
cpg	200.03	J/mol×K	634.90	Joback Method
cpg	206.95	J/mol×K	669.92	Joback Method
cpg	213.53	J/mol×K	704.95	Joback Method
cpg	219.76	J/mol×K	739.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R599803&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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