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

Other names:	Norfuraneol
	4-Hydroxy-5-methyl-3(2H)-dihydrofuranone
	3(2H)-Furanone, 4-hydroxy-5-methyl-
	4-hydroxy-5-methylfuran-3(2H)-one
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
CAS:	19322-27-1

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
rinpol	1087.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1054.00		NIST Webbook
ripol	2114.00		NIST Webbook
ripol	2123.00		NIST Webbook
ripol	2124.00		NIST Webbook
ripol	2114.00		NIST Webbook
ripol	2123.00		NIST Webbook
ripol	2120.00		NIST Webbook
ripol	2124.00		NIST Webbook
ripol	2105.00		NIST Webbook
ripol	2117.00		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

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=C19322271&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume