2(5H)-Furanone, 5-ethyl-3-hydroxy-4-methyl-

Other names:	5-Ethyl-3-hydroxy-4-methyl-2(5H)-furanone
	Abhexone
	2-Hexenoic acid, 2,4-dihydroxy-3-methyl-, «gamma»-lactone
	3-hydroxy-5-ethyl-4-methyl-2-(5H)-furanone
	5-Ethyl-4-methyl-3-hydroxy-2(5H)furanone
	5-Ethyl-3-hydroxy-4-methylfuran-2(5H)-one
	4-Methyl-5-ethyl-3-hydroxyfuranone
	Abhexon
	5-Ethyl-4-methyl-3-hydroxy-2(5H)furanone (Abhexone)
Inchi:	InChI=1S/C7H10O3/c1-3-5-4(2)6(8)7(9)10-5/h5,8H,3H2,1-2H3
InchiKey:	IUFQZPBIRYFPFD-UHFFFAOYSA-N
Formula:	C7H10O3
SMILES:	CCC1OC(=O)C(O)=C1C
Mol. weight [g/mol]:	142.15
CAS:	698-10-2

Physical Properties

Property code	Value	Unit	Source
gf	-290.22	kJ/mol	Joback Method
hf	-514.42	kJ/mol	Joback Method
hfus	19.84	kJ/mol	Joback Method
hvap	58.48	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	1.154		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
rinpol	1217.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1192.00		NIST Webbook

rinpol	1150.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1217.00		NIST Webbook
ripol	2260.00		NIST Webbook
ripol	2244.00		NIST Webbook
ripol	2246.00		NIST Webbook
ripol	2263.00		NIST Webbook
ripol	2267.00		NIST Webbook
ripol	2267.00		NIST Webbook
ripol	2260.00		NIST Webbook
ripol	2270.00		NIST Webbook
ripol	2250.00		NIST Webbook
ripol	2250.00		NIST Webbook
ripol	2247.00		NIST Webbook
ripol	2304.00		NIST Webbook
ripol	2304.00		NIST Webbook
ripol	2260.00		NIST Webbook
tb	570.91	K	Joback Method
tc	774.52	K	Joback Method
tf	360.96	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.78	J/mol×K	570.91	Joback Method
cpg	276.34	J/mol×K	604.85	Joback Method
cpg	286.45	J/mol×K	638.78	Joback Method
cpg	296.11	J/mol×K	672.72	Joback Method
cpg	305.30	J/mol×K	706.65	Joback Method
cpg	314.01	J/mol×K	740.59	Joback Method
cpg	322.24	J/mol×K	774.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C698102&Units=SI

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