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

Other names:	4-hydroxy-5-ethyl-2-methyl-3(2H)-furanone
	5-ethyl-4-hydroxy-2-methyl-3(2H)-furanone (EHMF)
	5-ethyl-4-hydroxy-2-methylfuran-3(2H)-one
Inchi:	InChI=1S/C7H10O3/c1-3-5-7(9)6(8)4(2)10-5/h4,9H,3H2,1-2H3
InchiKey:	QJYOEDXNPLUUAR-UHFFFAOYSA-N
Formula:	C7H10O3
SMILES:	CCC1=C(O)C(=O)C(C)O1
Mol. weight [g/mol]:	142.15
CAS:	27538-09-6

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	1140.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1140.00		NIST Webbook
ripol	2111.00		NIST Webbook
ripol	2111.00		NIST Webbook
ripol	2090.00		NIST Webbook
ripol	2080.00		NIST Webbook
ripol	2088.00		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: 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=C27538096&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