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

Inchi: InChI=1S/C7H10O3/c1-3-5-4(2)6(8)7(9)10-5/h6,8H,3H2,1-2H3
InchiKey: ZZWOFATXVNKRIR-UHFFFAOYSA-N
Formula: C7H10O3
SMILES: CCC1=C(C)C(O)C(=O)O1
Mol. weight [g/mol]: 142.15

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	-1.23		Crippen Method
logp	0.588		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
ripol	2277.00		NIST Webbook
ripol	2277.00		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=R390671&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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