

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

InChI: CC1=CC(=O)C(O)C1C
InChIKey: HGPVPAUYWUMPGW-UHFFFAOYSA-N

Formula: C7H12O3
SMILES: CCC1OC(C)C(O)C1=O
Mol. weight [g/mol]: 144.17

Physical Properties

Property code	Value	Unit	Source
gf	-316.34	kJ/mol	Joback Method
hf	-589.94	kJ/mol	Joback Method
hfus	21.54	kJ/mol	Joback Method
hvap	56.25	kJ/mol	Joback Method
log10ws	-0.61		Crippen Method
logp	0.114		Crippen Method
mcvol	111.940	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
rinpol	1145.00		NIST Webbook
rinpol	1145.00		NIST Webbook
ripol	2064.00		NIST Webbook
tb	552.45	K	Joback Method
tc	751.92	K	Joback Method
tf	326.68	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.94	J/molxK	552.45	Joback Method
cpg	302.87	J/molxK	585.69	Joback Method
cpg	315.25	J/molxK	618.94	Joback Method
cpg	327.08	J/molxK	652.18	Joback Method
cpg	338.34	J/molxK	685.43	Joback Method
cpg	349.02	J/molxK	718.67	Joback Method
cpg	359.10	J/molxK	751.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R303261&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rlnpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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