5-ethyl-5-methoxy-2(5 H)furanone

Inchi: InChI=1S/C7H10O3/c1-3-7(9-2)5-4-6(8)10-7/h4-5H,3H2,1-2H3
InchiKey: VZWSYQVRDZKYDD-UHFFFAOYSA-N
Formula: C7H10O3
SMILES: CCC1(OC)C=CC(=O)O1
Mol. weight [g/mol]: 142.15

Physical Properties

Property code	Value	Unit	Source
gf	-244.63	kJ/mol	Joback Method
hf	-456.23	kJ/mol	Joback Method
hfus	11.42	kJ/mol	Joback Method
hvap	41.74	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.852		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
rinpol	1080.00		NIST Webbook
tb	491.43	K	Joback Method
tc	714.96	K	Joback Method
tf	321.23	K	Joback Method
vc	0.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.90	J/mol×K	491.43	Joback Method
cpg	254.53	J/mol×K	528.69	Joback Method
cpg	266.44	J/mol×K	565.94	Joback Method
cpg	277.71	J/mol×K	603.20	Joback Method
cpg	288.40	J/mol×K	640.45	Joback Method
cpg	298.60	J/mol×K	677.71	Joback Method
cpg	308.38	J/mol×K	714.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R441551&Units=SI
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

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