5-ethyl-(3H)-furan-2-one

Other names: 2(3H)-Furanone, 5-ethyl-
5-Ethyldihydro-(3H)-furan-2-one
Inchi: InChI=1S/C6H8O2/c1-2-5-3-4-6(7)8-5/h3H,2,4H2,1H3
InchiKey: WWAGWEFPCZVKGN-UHFFFAOYSA-N
Formula: C6H8O2
SMILES: CCC1=CCC(=O)O1
Mol. weight [g/mol]: 112.13
CAS: 2313-01-1

Physical Properties

Property code	Value	Unit	Source
gf	-144.48	kJ/mol	Joback Method
hf	-309.74	kJ/mol	Joback Method
hfus	12.48	kJ/mol	Joback Method
hvap	39.23	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.227		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
ripol	1684.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1697.00		NIST Webbook
tb	455.54	K	Joback Method
tc	676.56	K	Joback Method
tf	280.59	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.63	J/mol×K	455.54	Joback Method
cpg	188.51	J/mol×K	492.38	Joback Method
cpg	198.93	J/mol×K	529.21	Joback Method
cpg	208.89	J/mol×K	566.05	Joback Method

cpg	218.38	J/mol×K	602.89	Joback Method
cpg	227.40	J/mol×K	639.72	Joback Method
cpg	235.94	J/mol×K	676.56	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=C2313011&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