2(3H)-Furanone, 5-ethylidenedihydro-

Inchi: InChI=1S/C6H8O2/c1-2-5-3-4-6(7)8-5/h2H,3-4H2,1H3/b5-2+
InchiKey: CBRZDGMGLYOALR-GORDUTHDSA-N
Formula: C6H8O2
SMILES: CC=C1CCC(=O)O1
Mol. weight [g/mol]: 112.13
CAS: 3393-34-8

Physical Properties

Property code	Value	Unit	Source
gf	-119.35	kJ/mol	Joback Method
hf	-280.02	kJ/mol	Joback Method
hfus	11.97	kJ/mol	Joback Method
hvap	39.06	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.227		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
rinpol	1325.00		NIST Webbook
rinpol	1325.00		NIST Webbook
tb	458.04	K	Joback Method
tc	683.52	K	Joback Method
tf	277.67	K	Joback Method
vc	0.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.76	J/mol×K	458.04	Joback Method
cpg	188.07	J/mol×K	495.62	Joback Method
cpg	198.87	J/mol×K	533.20	Joback Method
cpg	209.14	J/mol×K	570.78	Joback Method
cpg	218.89	J/mol×K	608.36	Joback Method
cpg	228.13	J/mol×K	645.94	Joback Method
cpg	236.85	J/mol×K	683.52	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=C3393348&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume