2(3H)-Furanone

Other names:	«alpha»-Crotonolactone
	«alpha»-Furanone
	«delta»,«beta»,«gamma»-Butenolide
	3-Butenoic acid, 4-hydroxy-, «gamma»-lactone
	2-Oxo-2,3-dihydrofuran
	«beta»,«gamma»-Crotonolactone
	2-Furanone
Inchi:	InChI=1S/C4H4O2/c5-4-2-1-3-6-4/h1,3H,2H2
InchiKey:	RHDGNLCLDBVESU-UHFFFAOYSA-N
Formula:	C4H4O2
SMILES:	O=C1CC=CO1
Mol. weight [g/mol]:	84.07
CAS:	20825-71-2

Physical Properties

Property code	Value	Unit	Source
gf	-151.69	kJ/mol	Joback Method
hf	-256.99	kJ/mol	Joback Method
hfus	7.69	kJ/mol	Joback Method
hvap	34.11	kJ/mol	Joback Method
ie	10.70	eV	NIST Webbook
log10ws	-0.60		Crippen Method
logp	0.447		Crippen Method
mcvol	59.500	ml/mol	McGowan Method
pc	5678.82	kPa	Joback Method
rinpol	914.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1726.00		NIST Webbook
tb	404.80	K	Joback Method
tc	630.37	K	Joback Method
tf	245.53	K	Joback Method
vc	0.215	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	103.50	J/mol×K	404.80	Joback Method
cpg	111.68	J/mol×K	442.39	Joback Method
cpg	119.51	J/mol×K	479.99	Joback Method
cpg	126.99	J/mol×K	517.58	Joback Method
cpg	134.12	J/mol×K	555.18	Joback Method
cpg	140.88	J/mol×K	592.77	Joback Method
cpg	147.27	J/mol×K	630.37	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20825712&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
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
ie: Ionization energy
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume