2,4(3H,5H)-Furandione

Other names:	Butanoic acid, 4-hydroxy-3-oxo-, «gamma»-lactone
	Tetronic acid
	Tetrahydrofuran-2,4-dione
	Tetrahydrofuran-3,5-dione
	Acetoacetic acid, 4-hydroxy-, «gamma»-lactone
	«beta»-oxo-«gamma»-butyrolactone
Inchi:	InChI=1S/C4H4O3/c5-3-1-4(6)7-2-3/h1-2H2
InchiKey:	JCGNDDUYTRNOFT-UHFFFAOYSA-N
Formula:	C4H4O3
SMILES:	O=C1COC(=O)C1
Mol. weight [g/mol]:	100.07
CAS:	4971-56-6

Physical Properties

Property code	Value	Unit	Source
gf	-304.24	kJ/mol	Joback Method
hf	-452.47	kJ/mol	Joback Method
hfus	5.98	kJ/mol	Joback Method
hvap	38.07	kJ/mol	Joback Method
log10ws	0.47		Crippen Method
logp	-0.498		Crippen Method
mcvol	65.370	ml/mol	McGowan Method
pc	5670.27	kPa	Joback Method
rinpol	833.00		NIST Webbook
rinpol	833.00		NIST Webbook
tb	473.46	K	Joback Method
tc	717.29	K	Joback Method
tf	312.99	K	Joback Method
vc	0.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	133.07	J/mol×K	473.46	Joback Method

cpg	142.43	J/mol×K	514.10	Joback Method
cpg	151.55	J/mol×K	554.74	Joback Method
cpg	160.37	J/mol×K	595.37	Joback Method
cpg	168.82	J/mol×K	636.01	Joback Method
cpg	176.87	J/mol×K	676.65	Joback Method
cpg	184.46	J/mol×K	717.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4971566&Units=SI

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