2(5H)-Furanone

Other names:	«gamma»-Crotonolactone
	«gamma»-Hydroxycrotonic acid lactone
	«delta»,«alpha»,«beta»-Butenolide
	Butenolide
	Isocrotonolactone
	2-Buten-4-olide
	2-Butenoic acid-«gamma»-lactone
	2-Butenoic acid, 4-hydroxy-, «gamma»-lactone
	2-Butenolide
	4-Hydroxy-2-butenoic acid «gamma»-lactone
	4-Hydroxy-2-butenoic acid lactone
	«gamma»-Crotolactone
	«alpha»,«beta»-Crotonolactone
	Crotonic acid, 4-hydroxy-, «gamma»-lactone
	2-Oxo-2,5-dihydrofuran
	5H-furan-2-one
	2,5-Dihydrofuranone
	NSC 197009
	Crotonolactone
	Furan-2(5H)-one
	2(5H)-Furanone («gamma»-crotonolactone)
Inchi:	InChI=1S/C4H4O2/c5-4-2-1-3-6-4/h1-2H,3H2
InchiKey:	VIHAEDVKXSOUAT-UHFFFAOYSA-N
Formula:	C4H4O2
SMILES:	O=C1C=CCO1
Mol. weight [g/mol]:	84.07
CAS:	497-23-4

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	55.60 ± 1.30	kJ/mol	NIST Webbook
log10ws	-0.11		Crippen Method
logp	0.099		Crippen Method

mcvol	59.500	ml/mol	McGowan Method
pc	5678.82	kPa	Joback Method
rinpol	863.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	915.60		NIST Webbook
ripol	1767.00		NIST Webbook
ripol	1787.00		NIST Webbook
ripol	1716.00		NIST Webbook
ripol	1716.00		NIST Webbook
ripol	1703.00		NIST Webbook
ripol	1692.00		NIST Webbook
ripol	1746.00		NIST Webbook
ripol	1702.00		NIST Webbook
ripol	1758.00		NIST Webbook
ripol	1787.00		NIST Webbook
ripol	1743.00		NIST Webbook
ripol	1742.00		NIST Webbook
ripol	1742.00		NIST Webbook
ripol	1742.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1712.00		NIST Webbook
ripol	1767.00		NIST Webbook
ripol	1745.00		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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.70	K	1.60	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C497234&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume