

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

Other names:	«alpha»-Methyl-«gamma»-crotonolactone 2-Methyl-2-butenolide 3-Methyl-2(5H)-furanone 2-Methyl-2-buten-4-olide
Inchi:	InChI=1S/C5H6O2/c1-4-2-3-7-5(4)6/h2H,3H2,1H3
InchiKey:	VGHBEMPMIVEGJP-UHFFFAOYSA-N
Formula:	C5H6O2
SMILES:	CC1=CCOC1=O
Mol. weight [g/mol]:	98.10
CAS:	22122-36-7

Physical Properties

Property code	Value	Unit	Source
gf	-152.90	kJ/mol	Joback Method
hf	-289.10	kJ/mol	Joback Method
hfus	9.89	kJ/mol	Joback Method
hvap	37.00	kJ/mol	Joback Method
log10ws	-0.53		Crippen Method
logp	0.489		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
pc	4835.95	kPa	Joback Method
rinpol	979.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	982.00		NIST Webbook
ripol	1759.00		NIST Webbook
ripol	1718.00		NIST Webbook
ripol	1713.00		NIST Webbook
ripol	1697.00		NIST Webbook
ripol	1718.00		NIST Webbook

ripol	1759.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1759.00		NIST Webbook
ripol	1682.00		NIST Webbook
ripol	1713.00		NIST Webbook
ripol	1713.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1694.00		NIST Webbook
ripol	1726.00		NIST Webbook
ripol	1683.00		NIST Webbook
ripol	1683.00		NIST Webbook
ripol	1683.00		NIST Webbook
tb	432.66	K	Joback Method
tc	656.90	K	Joback Method
tf	269.32	K	Joback Method
vc	0.272	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.67	J/mol×K	432.66	Joback Method
cpg	149.00	J/mol×K	470.03	Joback Method
cpg	157.97	J/mol×K	507.41	Joback Method
cpg	166.57	J/mol×K	544.78	Joback Method
cpg	174.79	J/mol×K	582.15	Joback Method
cpg	182.62	J/mol×K	619.53	Joback Method
cpg	190.05	J/mol×K	656.90	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=C22122367&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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