2(5H)-Furanone, 5,5-dimethyl-

Other names:	4,4-Dimethyl-2-buten-4-olide
	4,4-Dimethyl-2-butenolide
	4,4-Dimethylbut-2-enolide
	5,5-Dimethyl-2(5H)-furanone
	5,5-Dimethylbut-3-enolide
	5,5-Dimethylfuran-2(5H)-one
	4,4-Dimethylcrotonolactone
Inchi:	InChI=1S/C6H8O2/c1-6(2)4-3-5(7)8-6/h3-4H,1-2H3
InchiKey:	YNKQMZRTPPVLLL-UHFFFAOYSA-N
Formula:	C6H8O2
SMILES:	CC1(C)C=CC(=O)O1
Mol. weight [g/mol]:	112.13
CAS:	20019-64-1

Physical Properties

Property code	Value	Unit	Source
gf	-148.05	kJ/mol	Joback Method
hf	-303.37	kJ/mol	Joback Method
hfus	7.64	kJ/mol	Joback Method
hvap	37.11	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.878		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4403.25	kPa	Joback Method
rinpol	956.00		NIST Webbook
rinpol	907.50		NIST Webbook
rinpol	907.50		NIST Webbook
rinpol	907.50		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	951.70		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	951.70		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	946.00		NIST Webbook

rinpol	956.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	962.10		NIST Webbook
ripol	1590.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1590.00		NIST Webbook
ripol	1583.00		NIST Webbook
ripol	1583.00		NIST Webbook
tb	446.13	K	Joback Method
tc	675.56	K	Joback Method
tf	287.73	K	Joback Method
vc	0.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.23	J/mol×K	446.13	Joback Method
cpg	191.02	J/mol×K	484.37	Joback Method
cpg	201.97	J/mol×K	522.61	Joback Method
cpg	212.19	J/mol×K	560.84	Joback Method
cpg	221.76	J/mol×K	599.08	Joback Method
cpg	230.78	J/mol×K	637.32	Joback Method
cpg	239.35	J/mol×K	675.56	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20019641&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
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