2-Oxetanone, 3,3-dimethyl-

Other names:	«alpha»,«alpha»-Dimethyl-«beta»-propiolactone
	«alpha»,«alpha»-Dimethylpropiolactone
	Pivalic acid lactone
	Pivalolactone
	Propanoic acid, 3-hydroxy-2,2-dimethyl-, «beta»-lactone
	3,3-Dimethyl-«beta»-propiolactone
	3,3-Dimethyl-2-oxetanone
	NCI-C04126
	Hydracrylic acid, 2,2-dimethyl-, «beta»-lactone
	Pivalic acid, hydroxy-, lactone
Inchi:	InChI=1S/C5H8O2/c1-5(2)3-7-4(5)6/h3H2,1-2H3
InchiKey:	ULKFLOVGORAZDI-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	CC1(C)COC1=O
Mol. weight [g/mol]:	100.12
CAS:	1955-45-9

Physical Properties

Property code	Value	Unit	Source
chl	-2716.70	kJ/mol	NIST Webbook
gf	-174.33	kJ/mol	Joback Method
hf	-352.70	kJ/mol	NIST Webbook
hfl	-395.10	kJ/mol	NIST Webbook
hfus	5.93	kJ/mol	Joback Method
hvap	42.43	kJ/mol	NIST Webbook
hvap	42.40	kJ/mol	NIST Webbook
log10ws	-0.43		Crippen Method
logp	0.569		Crippen Method
mcvol	77.890	ml/mol	McGowan Method
pc	4615.13	kPa	Joback Method
tb	419.82	K	Joback Method
tc	640.67	K	Joback Method
tf	279.22	K	Joback Method
vc	0.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.68	J/mol×K	419.82	Joback Method
cpg	167.71	J/mol×K	456.63	Joback Method
cpg	177.94	J/mol×K	493.44	Joback Method
cpg	187.46	J/mol×K	530.25	Joback Method
cpg	196.36	J/mol×K	567.05	Joback Method
cpg	204.73	J/mol×K	603.86	Joback Method
cpg	212.66	J/mol×K	640.67	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=C1955459&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume