

Pivalolactone

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

Physical Properties

Property code	Value	Unit	Source
chl	-2716.70	kJ/mol	NIST Webbook
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
ie	10.02	eV	Cheméo Relay (1.0)
logp	0.569		Crippen Method
mcvol	77.890	ml/mol	McGowan 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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1955459&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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