

2,3-Dimethyl-4-hydroxy-2-butenolic lactone

Other names:	3,4-Dimethyl-2-butenolide 3,4-dimethyl-2(5H)-furanone
Inchi:	InChI=1S/C6H8O2/c1-4-3-8-6(7)5(4)2/h3H2,1-2H3
InchiKey:	QHQDWCHELGHSTO-UHFFFAOYSA-N
Formula:	C6H8O2
SMILES:	CC1=C(C)C(=O)OC1
Mol. weight [g/mol]:	112.13
CAS:	1575-46-8

Physical Properties

Property code	Value	Unit	Source
gf	-154.11	kJ/mol	Joback Method
hf	-321.21	kJ/mol	Joback Method
hfus	12.09	kJ/mol	Joback Method
hvap	39.89	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	0.880		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4167.71	kPa	Joback Method
ripol	1860.00		NIST Webbook
ripol	1844.00		NIST Webbook
ripol	1861.00		NIST Webbook
ripol	1862.00		NIST Webbook
tb	460.52	K	Joback Method
tc	682.96	K	Joback Method
tf	293.11	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.82	J/mol×K	460.52	Joback Method
cpg	188.25	J/mol×K	497.59	Joback Method
cpg	198.29	J/mol×K	534.67	Joback Method

cpg	207.94	J/mol×K	571.74	Joback Method
cpg	217.18	J/mol×K	608.81	Joback Method
cpg	226.00	J/mol×K	645.89	Joback Method
cpg	234.39	J/mol×K	682.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1575468&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/45-094-8/2-3-Dimethyl-4-hydroxy-2-butenic-lactone.pdf>

Generated by Cheméo on 2025-12-22 05:50:16.360373343 +0000 UTC m=+6130813.890413998.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.