

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

Other names:	.gamma.-butylbutyrolactone .gamma.-octalactone .gamma.-octanolactone 2(3H)-Furanone, dihydro-5-butyl- 4-Butyl-«gamma»-butyrolactone 4-Hydroxyoctanoic acid lactone 4-Hydroxyoctanoic acid, «gamma»-lactone 4-Octanolide 5-Butylidihydrofuran-2(3H)-one 5-Butyltetrahydro-2-furanone 5-butylidihydro-2(3H)-furanone NSC 24270 Octan-4-olide Octanoic acid, 4-hydroxy-, lactone Octanoic acid, 4-hydroxy-, «gamma»-lactone Octanoic acid, «gamma» lactone Octanolide-1,4 «gamma» -Octalactone «gamma»-Butyl-«gamma»-butyrolactone «gamma»-Butylbutyrolactone «gamma»-Octalactone «gamma»-Octanolactone «gamma»-n-Butyl-«gamma»-butyrolactone
Inchi:	InChI=1S/C8H14O2/c1-2-3-4-7-5-6-8(9)10-7/h7H,2-6H2,1H3
InchiKey:	IPBFYZQJXZJBFQ-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	CCCCC1CCC(=O)O1
Mol. weight [g/mol]:	142.20
CAS:	104-50-7

Physical Properties

Property code	Value	Unit	Source
gf	-155.68	kJ/mol	Joback Method
hf	-417.67	kJ/mol	Joback Method
hfus	17.90	kJ/mol	Joback Method
hvap	42.42	kJ/mol	Joback Method

log10ws	-2.04		Crippen Method
logp	1.882		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
rinpol	1210.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1215.00		NIST Webbook
rinpol	1225.00		NIST Webbook
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rinpol	1277.00		NIST Webbook
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ripol	1915.00	NIST Webbook
ripol	1943.00	NIST Webbook
ripol	1881.00	NIST Webbook
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ripol	1883.00	NIST Webbook

ripol	1940.00	NIST Webbook
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ripol	1946.00	NIST Webbook

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ripol	1912.00		NIST Webbook
ripol	1885.00		NIST Webbook
ripol	1906.00		NIST Webbook
ripol	1917.00		NIST Webbook
ripol	1910.00		NIST Webbook
ripol	1911.00		NIST Webbook
ripol	1881.00		NIST Webbook
ripol	1923.00		NIST Webbook
tb	492.49	K	Joback Method
tc	703.24	K	Joback Method
tf	285.61	K	Joback Method
vc	0.453	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.64	J/molxK	492.49	Joback Method
cpg	293.06	J/molxK	527.61	Joback Method
cpg	307.80	J/molxK	562.74	Joback Method
cpg	321.85	J/molxK	597.86	Joback Method
cpg	335.21	J/molxK	632.99	Joback Method
cpg	347.89	J/molxK	668.11	Joback Method
cpg	359.89	J/molxK	703.24	Joback Method
hvapt	66.00	kJ/mol	298.15	Vapor pressures and enthalpies of vaporization of a series of .gamma. and .delta.-lactones by correlation gas chromatography

Sources

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Vapor pressures and enthalpies of vaporization of a series of .gamma. and .delta.-lactones by correlation gas chromatography:

<https://www.doi.org/10.1016/j.jct.2014.01.016>

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=C104507&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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
hvapt: Enthalpy of vaporization at a given temperature
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

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