Butyrolactone

Other names:

2(3H)-Furanone, dihydro-
«gamma»-Butyrolactone
«gamma»-BL
«gamma»-Hydroxybutyric acid cyclic ester
«gamma»-Hydroxybutyric acid lactone
«gamma»-Hydroxybutyrolactone
Butanoic acid, 4-hydroxy-, «gamma»-lactone
Butyric acid lactone
Butyryl lactone
Dihydro-2(3H)-furanone
Tetrahydro-2-furanone
1,4-Butanolide
4-Butanolide
4-Butyrolactone
4-Deoxytetronic acid
4-Hydroxybutanoic acid lactone
4-Hydroxybutyric acid lactone
6480
1,4-Butyrolactone
«gamma»-6480
Butyric acid, 4-hydroxy-, «gamma»-lactone
Butyrylactone
BLO
BLON
Dihydro-2-furanone
NCI-C55878
1,2-Butanolide
4-Hydroxybutanoic acid, «gamma»-lactone
4-Hydroxybutyric acid, «gamma»-lactone
2-Oxolanone
1-Oxacyclopentan-2-one
2-Oxotetrahydrofuran
«gamma»-Butanolactone
«gamma»-Hydrooxybutyric acid lactone
Agrisynth BLO
GBL
Butyric acid, 4-hydroxy-, gamma-lactone
2(3H)-dihydrofuranone
Dihydro-(3 H)-furan-2-one
Dihydrofuran-2(3H)-one

NSC 4592
dihydro-2(3H)-furanone («gamma»-butyrolactone)
Butan-4-olide
Dihydro-2(3H)-furanone (-butyrolactone)
2-Dihydrofuranone

Inchi: InChI=1S/C4H6O2/c5-4-2-1-3-6-4/h1-3H2
InchiKey: YEJRWHAVMIAJKC-UHFFFAOYSA-N
Formula: C4H6O2
SMILES: O=C1CCCO1
Mol. weight [g/mol]: 86.09
CAS: 96-48-0

Physical Properties

Property code	Value	Unit	Source
affp	840.00	kJ/mol	NIST Webbook
basg	808.10	kJ/mol	NIST Webbook
chl	-2010.60 ± 0.50	kJ/mol	NIST Webbook
chl	-2012.46 ± 0.28	kJ/mol	NIST Webbook
chl	-2000.40 ± 6.40	kJ/mol	NIST Webbook
chl	-2009.20 ± 0.80	kJ/mol	NIST Webbook
gf	-181.65	kJ/mol	Joback Method
hf	-365.61 ± 0.44	kJ/mol	NIST Webbook
hf	-366.50 ± 0.80	kJ/mol	NIST Webbook
hf	-377.70	kJ/mol	NIST Webbook
hf	-368.50	kJ/mol	NIST Webbook
hf	-364.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-431.20 ± 2.70	kJ/mol	NIST Webbook
hfl	-419.07 ± 0.36	kJ/mol	NIST Webbook
hfl	-420.90 ± 0.70	kJ/mol	NIST Webbook
hfl	-419.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-422.00 ± 1.10	kJ/mol	NIST Webbook
hfus	6.47	kJ/mol	Joback Method
hvap	47.60 ± 4.00	kJ/mol	NIST Webbook
hvap	53.10 ± 0.20	kJ/mol	NIST Webbook
hvap	48.00 ± 0.40	kJ/mol	NIST Webbook
hvap	55.00 ± 1.00	kJ/mol	NIST Webbook
hvap	55.00	kJ/mol	NIST Webbook
hvap	55.20 ± 1.30	kJ/mol	NIST Webbook
hvap	55.60 ± 1.40	kJ/mol	NIST Webbook
hvap	54.40 ± 0.40	kJ/mol	NIST Webbook

hvap	54.40	kJ/mol	NIST Webbook
hvap	54.40 ± 0.40	kJ/mol	NIST Webbook
hvap	54.60 ± 0.20	kJ/mol	NIST Webbook
hvap	51.50	kJ/mol	NIST Webbook
hvap	48.90 ± 0.30	kJ/mol	NIST Webbook
hvap	53.46 ± 0.13	kJ/mol	NIST Webbook
hvap	53.50	kJ/mol	NIST Webbook
hvap	54.90 ± 0.20	kJ/mol	NIST Webbook
ie	10.26	eV	NIST Webbook
ie	10.26	eV	NIST Webbook
log10ws	-0.25		Crippen Method
logp	0.323		Crippen Method
mcvol	63.800	ml/mol	McGowan Method
pc	5131.00 ± 40.00	kPa	NIST Webbook
rinpol	911.00		NIST Webbook
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ripol	1636.00		NIST Webbook
ripol	1635.00		NIST Webbook
ripol	1611.00		NIST Webbook
sl	197.40	J/mol×K	NIST Webbook
sl	201.28	J/mol×K	NIST Webbook
sl	197.50	J/mol×K	NIST Webbook
tb	477.70	K	NIST Webbook
tb	479.20 ± 0.20	K	NIST Webbook
tc	731.00 ± 0.40	K	NIST Webbook
tf	229.00 ± 0.60	K	NIST Webbook
tt	229.78 ± 0.05	K	NIST Webbook
tt	229.78 ± 0.02	K	NIST Webbook
tt	229.78 ± 0.01	K	NIST Webbook
vc	0.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.61	J/mol×K	554.37	Joback Method

cpg	160.69	J/mol×K	591.56	Joback Method
cpg	116.24	J/mol×K	405.64	Joback Method
cpg	125.93	J/mol×K	442.82	Joback Method
cpg	135.22	J/mol×K	480.01	Joback Method
cpg	144.12	J/mol×K	517.19	Joback Method
cpg	168.36	J/mol×K	628.74	Joback Method
cpl	141.30	J/mol×K	298.15	NIST Webbook
cpl	141.40	J/mol×K	298.15	NIST Webbook
cpl	140.50	J/mol×K	298.15	NIST Webbook
cpl	140.90	J/mol×K	298.15	NIST Webbook
cpl	141.30	J/mol×K	298.15	NIST Webbook
hfust	9.57	kJ/mol	229.78	NIST Webbook
hfust	9.57	kJ/mol	230.00	NIST Webbook
hfust	9.57	kJ/mol	229.78	NIST Webbook
hvapt	45.20 ± 0.40	kJ/mol	349.00	NIST Webbook
hvapt	48.20	kJ/mol	433.00	NIST Webbook
hvapt	49.50 ± 0.10	kJ/mol	392.00	NIST Webbook
hvapt	51.80 ± 0.60	kJ/mol	357.50	NIST Webbook
sfust	41.56	J/mol×K	229.78	NIST Webbook
sfust	41.56	J/mol×K	229.78	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.20	K	1.60	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C96480&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

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume