

2-Oxetanone, 4-methyl-

Other names:	.beta.-butyrolactone .beta.-methyl-.beta.-propiolactone .beta.-methylpropiolactone 2-butenic lactone 3-Hydroxybutanoic acid, «beta»-lactone 3-Hydroxybutyric acid, «beta»-lactone 3-butanolide 3-hydroxybutyric acid .beta.-lactone 3-hydroxybutyric acid lactone 3-methyl-3-propiolactone 4-methyl-2-oxetanone 4-methyloxetan-2-one Butanoic acid, 3-hydroxy-, beta-lactone DL-«beta»-Butyrolactone Hydroxybutyric acid lactone butanoic acid, 3-hydroxy-, .beta.-lactone butyric acid, 3-hydroxy-, .beta.-lactone «beta»-Butyrolactone «beta»-Butyrolakton
Inchi:	InChI=1S/C4H6O2/c1-3-2-4(5)6-3/h3H,2H2,1H3
InchiKey:	GSCLMSFRWBPUK-UHFFFAOYSA-N
Formula:	C4H6O2
SMILES:	CC1CC(=O)O1
Mol. weight [g/mol]:	86.09
CAS:	3068-88-0

Physical Properties

Property code	Value	Unit	Source
gf	-177.26	kJ/mol	Joback Method
hf	-328.95	kJ/mol	Joback Method
hfus	9.64	kJ/mol	Joback Method
hvap	33.34	kJ/mol	Joback Method
log10ws	-0.37		Crippen Method
logp	0.322		Crippen Method
mcvol	63.800	ml/mol	McGowan Method
pc	4952.36	kPa	Joback Method
tb	396.70	K	Joback Method

tc	609.99	K	Joback Method
tf	244.05	K	Joback Method
vc	0.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	119.74	J/molxK	396.70	Joback Method
cpg	161.68	J/molxK	574.44	Joback Method
cpg	153.96	J/molxK	538.89	Joback Method
cpg	145.91	J/molxK	503.34	Joback Method
cpg	137.52	J/molxK	467.80	Joback Method
cpg	128.80	J/molxK	432.25	Joback Method
cpg	169.04	J/molxK	609.99	Joback Method
speedsl	1263.57	m/s	323.15	A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones
speedsl	1281.08	m/s	318.15	A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones
speedsl	1298.78	m/s	313.15	A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones
speedsl	1316.65	m/s	308.15	A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones

speedsl	1334.65	m/s	303.15	A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones
speedsl	1352.77	m/s	298.15	A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones
speedsl	1371.04	m/s	293.15	A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3068880&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones:	https://www.doi.org/10.1016/j.jct.2016.12.032
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
speedsl:	Speed of sound in fluid

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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