2-Oxetanone, 4-methyl-

Other names:	.betabutyrolactone
	.betamethylbetapropiolactone
	.betamethylpropiolactone
	2-butenoic lactone
	3-Hydroxybutanoic acid, «beta»-lactone
	3-Hydroxybutyric acid, «beta»-lactone
	3-butanolide
	3-hydroxybutyric acid .betalactone
	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-, .betalactone
	butyric acid, 3-hydroxy-, .betalactone
	«beta»-Butyrolactone
	«beta»-Butyrolakton
Inchi:	InChI=1S/C4H6O2/c1-3-2-4(5)6-3/h3H,2H2,1H3
InchiKey:	GSCLMSFRWBPUSK-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
рс	4952.36	kPa	Joback Method
tb	396.70	K	Joback Method

tc	609.99	К	Joback Method
tf	244.05	К	Joback Method
VC	0.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K] Source	
cpg	119.74	J/mol×K	396.70	Joback Method	
cpg	161.68	J/mol×K	574.44	Joback Method	
cpg	153.96	J/mol×K	538.89	Joback Method	
cpg	145.91	J/mol×K	503.34	Joback Method	
cpg	137.52	J/mol×K	467.80	Joback Method	
cpg	128.80	J/mol×K	432.25	Joback Method	
cpg	169.04	J/mol×K	609.99	Joback Method	
speedsl	1263.57	m/s	323.15 s	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 s	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 s	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 s	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

A comparative study on the interactions of [bmim][NTf2] ionic llqbrcwMeterected four- to seven-membered-ring lactones: McGowan Method:	https://www.doi.org/10.1016/j.jct.2016.12.032 https://en.wikipedia.org/wiki/Joback_method http://link.springer.com/article/10.1007/BF02311772
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

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
рс:	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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