

# 2-Ethyl-2-hydroxybutyric acid

<b>Other names:</b>	Butanoic acid, 2-ethyl-2-hydroxy-
<b>Inchi:</b>	InChI=1S/C6H12O3/c1-3-6(9,4-2)5(7)8/h9H,3-4H2,1-2H3,(H,7,8)
<b>InchiKey:</b>	LXVSANCQXSSLPA-UHFFFAOYSA-N
<b>Formula:</b>	C6H12O3
<b>SMILES:</b>	CCC(O)(CC)C(=O)O
<b>Mol. weight [g/mol]:</b>	132.16
<b>CAS:</b>	3639-21-2

## Physical Properties

Property code	Value	Unit	Source
gf	-400.08	kJ/mol	Joback Method
hf	-592.96	kJ/mol	Joback Method
hfus	13.66	kJ/mol	Joback Method
hvap	67.76	kJ/mol	Joback Method
log10ws	-0.81		Crippen Method
logp	0.622		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	4283.05	kPa	Joback Method
tb	571.68	K	Joback Method
tc	745.53	K	Joback Method
tf	331.37	K	Joback Method
vc	0.405	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.59	J/molxK	571.68	Joback Method
cpg	279.74	J/molxK	600.66	Joback Method
cpg	287.45	J/molxK	629.63	Joback Method
cpg	294.75	J/molxK	658.61	Joback Method
cpg	301.65	J/molxK	687.58	Joback Method
cpg	308.18	J/molxK	716.56	Joback Method
cpg	314.36	J/molxK	745.53	Joback Method
dvisc	0.0218901	Paxs	331.37	Joback Method

dvisc	0.0045887	Paxs	371.42	Joback Method
dvisc	0.0013039	Paxs	411.47	Joback Method
dvisc	0.0004632	Paxs	451.52	Joback Method
dvisc	0.0001947	Paxs	491.58	Joback Method
dvisc	0.0000933	Paxs	531.63	Joback Method
dvisc	0.0000496	Paxs	571.68	Joback Method

## Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3639212&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3639212&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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