

# Butanoic acid, 2,2-diethyl-

<b>Inchi:</b>	InChI=1S/C8H16O2/c1-4-8(5-2,6-3)7(9)10/h4-6H2,1-3H3,(H,9,10)
<b>InchiKey:</b>	GHXNRYVDXNZID-UHFFFAOYSA-N
<b>Formula:</b>	C8H16O2
<b>SMILES:</b>	CCC(CC)(CC)C(=O)O
<b>Mol. weight [g/mol]:</b>	144.21
<b>CAS:</b>	813-58-1

## Physical Properties

Property code	Value	Unit	Source
gf	-246.42	kJ/mol	Joback Method
hf	-482.01	kJ/mol	Joback Method
hfus	14.75	kJ/mol	Joback Method
hvap	55.53	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	2.287		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
tb	525.26	K	Joback Method
tc	703.40	K	Joback Method
tf	312.15 ± 2.00	K	NIST Webbook
vc	0.497	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.82	J/molxK	525.26	Joback Method
cpg	324.40	J/molxK	554.95	Joback Method
cpg	335.40	J/molxK	584.64	Joback Method
cpg	345.83	J/molxK	614.33	Joback Method
cpg	355.72	J/molxK	644.02	Joback Method
cpg	365.10	J/molxK	673.71	Joback Method
cpg	373.98	J/molxK	703.40	Joback Method
dvisc	0.0196912	Paxs	293.09	Joback Method
dvisc	0.0053599	Paxs	331.79	Joback Method

dvisc	0.0019147	Paxs	370.48	Joback Method
dvisc	0.0008310	Paxs	409.18	Joback Method
dvisc	0.0004166	Paxs	447.87	Joback Method
dvisc	0.0002331	Paxs	486.56	Joback Method
dvisc	0.0001421	Paxs	525.26	Joback Method

## Sources

<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=C813581&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C813581&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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