

# Butyric acid, 4,4,4-trinitro-, ethyl ester

<b>Inchi:</b>	InChI=1S/C6H9N3O8/c1-2-17-5(10)3-4-6(7(11)12,8(13)14)9(15)16/h2-4H2,1H3
<b>InchiKey:</b>	FUAMTTZWZQPBF5-UHFFFAOYSA-N
<b>Formula:</b>	C6H9N3O8
<b>SMILES:</b>	CCOC(=O)CCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	251.15
<b>CAS:</b>	15421-42-8

## Physical Properties

Property code	Value	Unit	Source
chl	-3133.00	kJ/mol	NIST Webbook
gf	-124.79	kJ/mol	Joback Method
hf	-453.00	kJ/mol	Joback Method
hfus	40.75	kJ/mol	Joback Method
hvap	86.58	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	-0.186		Crippen Method
mcvol	155.100	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
tb	865.26	K	Joback Method
tc	1125.47	K	Joback Method
tf	662.79	K	Joback Method
vc	0.630	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.19	J/molxK	865.26	Joback Method
cpg	462.96	J/molxK	908.63	Joback Method
cpg	469.86	J/molxK	952.00	Joback Method
cpg	475.95	J/molxK	995.36	Joback Method
cpg	481.29	J/molxK	1038.73	Joback Method
cpg	485.94	J/molxK	1082.10	Joback Method
cpg	489.98	J/molxK	1125.47	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=C15421428&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C15421428&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<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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