

# Butanoic acid, 2-ethyl-, methyl ester

<b>Other names:</b>	2-Ethylbutyric acid, methyl ester Butyric acid, 2-ethyl-, methyl ester Methyl 2-ethylbutanoate Methyl 2-ethylbutyrate
<b>Inchi:</b>	InChI=1S/C7H14O2/c1-4-6(5-2)7(8)9-3/h6H,4-5H2,1-3H3
<b>InchiKey:</b>	UNEAEGWIVFZPFI-UHFFFAOYSA-N
<b>Formula:</b>	C7H14O2
<b>SMILES:</b>	CCC(CC)C(=O)OC
<b>Mol. weight [g/mol]:</b>	130.18
<b>CAS:</b>	816-11-5

## Physical Properties

Property code	Value	Unit	Source
gf	-228.30	kJ/mol	Joback Method
hf	-437.89	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	39.94	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.596		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	845.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	845.00		NIST Webbook
tb	435.41	K	Joback Method
tc	615.76	K	Joback Method
tf	225.81	K	Joback Method
vc	0.446	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.73	J/molxK	435.41	Joback Method

cpg	250.17	J/molxK	465.47	Joback Method
cpg	261.22	J/molxK	495.53	Joback Method
cpg	271.87	J/molxK	525.58	Joback Method
cpg	282.12	J/molxK	555.64	Joback Method
cpg	291.98	J/molxK	585.70	Joback Method
cpg	301.45	J/molxK	615.76	Joback Method
dvisc	0.0047724	Paxs	225.81	Joback Method
dvisc	0.0021099	Paxs	260.74	Joback Method
dvisc	0.0011312	Paxs	295.68	Joback Method
dvisc	0.0006919	Paxs	330.61	Joback Method
dvisc	0.0004649	Paxs	365.54	Joback Method
dvisc	0.0003348	Paxs	400.48	Joback Method
dvisc	0.0002542	Paxs	435.41	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44632e+01
Coeff. B	-3.53578e+03
Coeff. C	-5.48940e+01
Temperature range (K), min.	304.32
Temperature range (K), max.	441.24

## Sources

**The Yaws Handbook of Vapor**

**Pressure:**  
**Crippen Method:**

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C816115&Units=SI>

## 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>pvap:</b>	Vapor pressure
<b>rinpola:</b>	Non-polar retention indices
<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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