

# Benzoic acid, 4-ethyl-, methyl ester

<b>Other names:</b>	4-Ethylbenzoic acid, methyl ester
<b>Inchi:</b>	InChI=1S/C10H12O2/c1-3-8-4-6-9(7-5-8)10(11)12-2/h4-7H,3H2,1-2H3
<b>InchiKey:</b>	CAABRJFUDNBRJZ-UHFFFAOYSA-N
<b>Formula:</b>	C10H12O2
<b>SMILES:</b>	CCc1ccc(C(=O)OC)cc1
<b>Mol. weight [g/mol]:</b>	164.20
<b>CAS:</b>	7364-20-7

## Physical Properties

Property code	Value	Unit	Source
gf	-97.82	kJ/mol	Joback Method
hf	-269.47	kJ/mol	Joback Method
hfus	18.10	kJ/mol	Joback Method
hvap	49.95	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.036		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
rinpol	1325.80		NIST Webbook
tb	536.15	K	Joback Method
tc	749.95	K	Joback Method
tf	313.56	K	Joback Method
vc	0.511	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.27	J/molxK	536.15	Joback Method
cpg	313.54	J/molxK	571.78	Joback Method
cpg	326.10	J/molxK	607.42	Joback Method
cpg	337.97	J/molxK	643.05	Joback Method
cpg	349.15	J/molxK	678.68	Joback Method
cpg	359.66	J/molxK	714.31	Joback Method
cpg	369.52	J/molxK	749.95	Joback Method

dvisc	0.0017515	Paxs	313.56	Joback Method
dvisc	0.0010200	Paxs	350.66	Joback Method
dvisc	0.0006587	Paxs	387.76	Joback Method
dvisc	0.0004592	Paxs	424.86	Joback Method
dvisc	0.0003392	Paxs	461.95	Joback Method
dvisc	0.0002621	Paxs	499.05	Joback Method
dvisc	0.0002099	Paxs	536.15	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=C7364207&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7364207&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>rinpol:</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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