

# Benzoic acid, 4-bromo-, ethyl ester

<b>Other names:</b>	Benzoic acid, p-bromo-, ethyl ester p-(Ethoxycarbonyl)phenyl bromide Ethyl p-bromobenzoate Ethyl-4-bromobenzoate 4-Bromobenzoic acid, ethyl ester
<b>Inchi:</b>	InChI=1S/C9H9BrO2/c1-2-12-9(11)7-3-5-8(10)6-4-7/h3-6H,2H2,1H3
<b>InchiKey:</b>	XZIAFENWXIQUIKR-UHFFFAOYSA-N
<b>Formula:</b>	C9H9BrO2
<b>SMILES:</b>	CCOC(=O)c1ccc(Br)cc1
<b>Mol. weight [g/mol]:</b>	229.07
<b>CAS:</b>	5798-75-4

## Physical Properties

Property code	Value	Unit	Source
gf	-91.92	kJ/mol	Joback Method
hf	-222.50	kJ/mol	Joback Method
hfus	20.79	kJ/mol	Joback Method
hvap	54.16	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.626		Crippen Method
mcvol	138.850	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	579.43	K	Joback Method
tc	811.07	K	Joback Method
tf	362.09	K	Joback Method
vc	0.517	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.08	J/molxK	579.43	Joback Method
cpg	340.71	J/molxK	772.46	Joback Method
cpg	332.17	J/molxK	733.85	Joback Method
cpg	322.96	J/molxK	695.25	Joback Method

cpg	313.06	J/molxK	656.64	Joback Method
cpg	302.44	J/molxK	618.04	Joback Method
cpg	348.60	J/molxK	811.07	Joback Method
dvisc	0.0002365	Paxs	579.43	Joback Method
dvisc	0.0002908	Paxs	543.21	Joback Method
dvisc	0.0003681	Paxs	506.98	Joback Method
dvisc	0.0004832	Paxs	470.76	Joback Method
dvisc	0.0006638	Paxs	434.54	Joback Method
dvisc	0.0009661	Paxs	398.31	Joback Method
dvisc	0.0015157	Paxs	362.09	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	535.20	K	98.30	NIST Webbook
tbrp	535.00	K	98.30	NIST Webbook
tbrp	404.00	K	1.70	NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>
<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=C5798754&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5798754&amp;Units=SI</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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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