

# (E)-But-2-enyl 3-chlorobenzoate

<b>Other names:</b>	Benzoic acid, 3-chloro, (E)-2-butenyl ester
<b>Inchi:</b>	InChI=1S/C11H11ClO2/c1-2-3-7-14-11(13)9-5-4-6-10(12)8-9/h2-6,8H,7H2,1H3/b3-2+
<b>InchiKey:</b>	YSMHCWQQKGGAGR-NSCUHMNNSA-N
<b>Formula:</b>	C11H11ClO2
<b>SMILES:</b>	CC=CCOC(=O)c1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	210.66

## Physical Properties

Property code	Value	Unit	Source
gf	-21.11	kJ/mol	Joback Method
hf	-188.63	kJ/mol	Joback Method
hfus	25.08	kJ/mol	Joback Method
hvap	56.52	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.073		Crippen Method
mcvol	157.470	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1530.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1521.00		NIST Webbook
ripol	2158.00		NIST Webbook
ripol	2133.00		NIST Webbook
ripol	2152.00		NIST Webbook
ripol	2172.00		NIST Webbook
ripol	2174.00		NIST Webbook
ripol	2147.00		NIST Webbook
tb	600.62	K	Joback Method
tc	824.35	K	Joback Method
tf	349.67	K	Joback Method
vc	0.597	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.29	J/molxK	600.62	Joback Method
cpg	364.97	J/molxK	637.91	Joback Method
cpg	376.83	J/molxK	675.20	Joback Method
cpg	387.90	J/molxK	712.49	Joback Method
cpg	398.21	J/molxK	749.77	Joback Method
cpg	407.80	J/molxK	787.06	Joback Method
cpg	416.70	J/molxK	824.35	Joback Method
dvisc	0.0014831	Paxs	349.67	Joback Method
dvisc	0.0008442	Paxs	391.50	Joback Method
dvisc	0.0005358	Paxs	433.32	Joback Method
dvisc	0.0003684	Paxs	475.14	Joback Method
dvisc	0.0002691	Paxs	516.97	Joback Method
dvisc	0.0002060	Paxs	558.79	Joback Method
dvisc	0.0001637	Paxs	600.62	Joback Method

## Sources

<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=U373543&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U373543&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>ripol:</b>	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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