Benzoic acid, 3-chloro-, ethyl ester

Other names:	Benzoic acid, m-chloro-, ethyl ester
	Ethyl m-chlorobenzoate
	Ethyl 3-chlorobenzoate
	3-Chlorobenzoic acid, ethyl ester
Inchi:	InChI=1S/C9H9ClO2/c1-2-12-9(11)7-4-3-5-8(10)6-7/h3-6H,2H2,1H3
InchiKey:	LVFRSNCBCHABAM-UHFFFAOYSA-N
Formula:	C9H9ClO2
SMILES:	CCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]:	184.62
CAS:	1128-76-3

Physical Properties

Property code	Value	Unit	Source
gf	-118.17	kJ/mol	Joback Method
hf	-264.57	kJ/mol	Joback Method
hfus	19.70	kJ/mol	Joback Method
hvap	52.11	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.517		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
rinpol	1340.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1314.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1314.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1318.00		NIST Webbook

ripol	1832.00		NIST Webbook
ripol	1850.00		NIST Webbook
ripol	1887.00		NIST Webbook
ripol	1893.00		NIST Webbook
ripol	1909.00		NIST Webbook
ripol	1863.00		NIST Webbook
ripol	1863.00		NIST Webbook
tb	550.70	K	Joback Method
tc	772.80	K	Joback Method
tf	332.21	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.82	J/mol×K	550.70	Joback Method
cpg	292.35	J/mol×K	587.72	Joback Method
cpg	303.20	J/mol×K	624.73	Joback Method
cpg	313.39	J/mol×K	661.75	Joback Method
cpg	322.92	J/mol×K	698.76	Joback Method
cpg	331.82	J/mol×K	735.78	Joback Method
cpg	340.09	J/mol×K	772.80	Joback Method
dvisc	0.0016956	Pa×s	332.21	Joback Method
dvisc	0.0010290	Pa×s	368.63	Joback Method
dvisc	0.0006831	Pa×s	405.04	Joback Method
dvisc	0.0004852	Pa×s	441.46	Joback Method
dvisc	0.0003631	Pa×s	477.87	Joback Method
dvisc	0.0002831	Pa×s	514.29	Joback Method
dvisc	0.0002281	Pa×s	550.70	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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=C1128763&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume